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Optimization and economic analysis of energetic systems in a wastewater treatment plant

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Optimization and economic analysis of energetic systems in a wastewater treatment plant

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Abstract

The main purpose of this work was the development of energy optimization procedures for a wastewater treatment plant. Along with it, solutions were presented and analysed for economic viability. For this aim, extensive bibliographic research was undertaken to better understand the existing tools, models, and results already achieved with each set of conditions.

To elaborate the case-study, data for biogas production and electricity needs of a wastewater treatment plant were retrieve. Alongside it, the Solcast API was utilized to retrieve historical data.

After schematizing the functioning of the plant, a rule-based approach was selected for the simulation and optimization of energy. To guide the programming, flowcharts were designed to mimic the relations between each set of variables and components. With the intent of making the simulator have a more widespread utilization, the required programming was executed in Excel and VBA (Visual Basic for Applications).

The results were broken down and analysed with the objectives of burnt biogas minimization, cost reduction, and self-sufficiency in view. Results showed a vast improvement after the introduction of the energy optimization system, with self-sustainability ratio increasing from 70% to above 91% in all analysed scenarios with both biogas and photovoltaic as renewable energy sources.

The implementation of a secondary cogeneration unit was studied, to reduce the amount of burnt biogas in low-purchase scenarios. Results showed that the application of a second cogeneration unit can be profitable, if the wasted biogas is close to 25% of the total production. Similarly, the cost-effectiveness of the implementation of the photovoltaic system was also analysed, due to the high amount of exceeding energy derived from this source of energy. Two solutions were tested. The first one showed that establishing a renewable energy community with neighbouring facilities is a viable alternative to utilize the excess of produced electricity, with the internal rate of return oscillating between 38.68% and 15.45%, depending on the simulation scenario. The second analysis consisted of a sensitivity analysis of the selling price of electricity. It utilized the scenario which yielded the worst result on the previous analysis. It determined that, for selling prices higher than 0.15 €/kWh, it can be a viable option to sell the electricity back to the grid, even though it does not achieve the same economic benefits as the community approach.

Keywords: Self-sustainability, Renewable energy community, Wastewater treatment plant, Optimization, Multi-energy system

Resumo

O principal objetivo deste trabalho foi o desenvolvimento de procedimentos de otimização energética para uma estação de tratamento de águas residuais. Foram apresentadas soluções e analisada a sua viabilidade económica. Para o efeito, foi efetuada uma extensa pesquisa bibliográfica para melhor conhecer as ferramentas, modelos e resultados existentes já alcançados com cada conjunto de condições.

Para elaborar o caso de estudo, foram utilizados dados relativos à produção de biogás e às necessidades de eletricidade de uma estação de tratamento de águas residuais. Foi utilizada a API Solcast para obter dados históricos de irradiância para o ano de 2023.

Após esquematizar o funcionamento da estação, foi selecionada uma abordagem baseada em regras para a simulação e otimização da energia. Para guiar a programação, foram desenhados fluxogramas que simulam as relações entre cada conjunto de variáveis e componentes. Com o objetivo de generalizar a utilização do simulador, a programação necessária foi executada em Excel e VBA (*Visual Basic for Applications*).

Os resultados foram decompostos e analisados tendo em vista os objetivos de minimização do biogás queimado, redução de custos e autossuficiência. Foram desenhados quatro cenários de otimização: dois com o objetivo de atingir um compromisso entre a diminuição do biogás queimado e a poupança económica, sendo que um utiliza apenas os dados referentes à produção de biogás e às necessidades energéticas da estação de tratamento de águas residuais, e o outro adiciona os dados referentes à produção de energia com recurso ao sistema fotovoltaico; um com o objetivo singular de minimizar a queima de biogás; e um último com o objetivo de reduzir a quantidade de energia adquirida. Cada um dos cenários apresentou resultados superiores aos existentes sem otimização para os fins a que se destinava. Dois cenários conseguiram evitar a queima de biogás durante um ano. Por outro lado, e apesar de nenhum dos cenários ter conseguido evitar a compra de eletricidade à rede elétrica, os custos foram substancialmente minimizados. O caso dedicado à minimização de compra de eletricidade conseguiu, durante um ano, adquirir apenas 23,818.30 kWh de energia, o que equivale, de acordo com a estimativa, a 2,446.14 €. Os resultados mostraram uma grande melhoria após a introdução do sistema de otimização energética, com o rácio de autossustentabilidade a aumentar de 70% para mais de 91% em todos os cenários analisados que utilizam biogás e fotovoltaico como fontes de energias renováveis.

Foi estudada a implementação de uma unidade de cogeração secundária, para reduzir a quantidade de biogás queimado em cenários de baixa compra. Os resultados mostraram que a aplicação de uma segunda unidade de cogeração pode ser rentável se o biogás desperdiçado estiver próximo dos 25% da produção total. Do mesmo modo, foi também analisada a relação custo-eficácia da implementação do sistema fotovoltaico, devido à elevada quantidade de energia excedentária derivada desta fonte de energia. Foram testadas duas soluções. A primeira mostrou que a criação de uma comunidade de energia renovável com instalações vizinhas é uma alternativa viável para utilizar o excesso de eletricidade produzida, com a taxa interna de retorno a oscilar entre 38.68% e 15.45%, dependendo do cenário de simulação. A segunda análise consistiu numa análise de sensibilidade ao preço de venda da eletricidade. Utilizou-se o cenário que apresentou o pior resultado na análise anterior. Determinou-se que, para preços de venda superiores a 0,15 €/kWh, pode ser uma opção viável vender a eletricidade de volta à rede, apesar de não se obter os mesmos benefícios económicos que a abordagem comunitária.

Palavras-chave: Autossustentabilidade, Comunidades de energia renovável, Estação de tratamento de águas residuais, Otimização, Sistemas multi-energia

Contents

List of Figures

List of Tables

Abbreviations and symbols

List of abbreviations

ADENE	*Agência para a Energia*
AEMs	Actual Engineering Models
AI	Artificial Intelligence
ANN	Artificial Neural Network
API	Application Programming Interface
BDD	Boron-dropped Diamond
BPNN	Back Propagation Neural Networks
CAD	Computer-aided Design
CCHP	Combined Heat, Cold, and Power
CHP	Combined Heat and Power
CO2	Carbon Dioxide
CRP	Capital Recovery Period
CT	Cooling Tower
DBN	Deep Belief Network
DDPG	Deep Deterministic Policy Gradient
DERMs	Distribution Energy Resource Management
DERMS	Distribution Energy Resource Management Systems
DERs	Distribution Energy Resource
DES	Discrete Event Simulation
DL	Deep Learning
DNN	Deep Neural Networks

DR	Deep Reinforcement
DRL	Deep Reinforcement Learning
DRO	Distributionally Robust Optimization
DRP	Demand Response Programs
DRWNN	Diagonal Recurrent Wavelet Neural Networks
EH	Energy Hub
ERSE	*Entidade Reguladora dos Serviços de Energia*
EU	European Union
EV	Electrical Vehicles
FNN	Feedforward Neural Network
GA	Genetic Algorithm
GAMS	General Algebraic Modelling System
GAN	Generative Adversarial Network
GHG	Greenhouse Gas
GHI	Global Horizontal Irradiance
GWh	Gigawatt Hours
HOA	Hybrid Optimization Algorithm
HOMER	Hybrid Optimization of Multiple Energy Resources
IEA	International Energy Agency
IES	Integrated Energy System
IRR	Internal Rate of Return
KPI	Key Performance Indicator
LSTM	Long Short-term Memorie
MCA	Multi-Criteria Analysis

MCS	Monte Carlo Simulation
MES	Multi-energy System
MILP	Mixed-integer Linear Programming
ML	Machine Learning
MW	Megawatt
MWh	Megawatt hours
NPV	Net Present Value
NREL	National Renewable Energy Laboratory
PAI	Plane of Array Irradiation
PDF	Probability Density Functions
PEM	Point Estimate Method
PM	Persistence Model
PSEO	Photovoltaic Solar Electro-oxidation
PV	Photovoltaic
PVL	Photovoltaic Load
REC	Renewable Energy Communities
ReLU	Rectified Linear Unit
RES	Renewable Energy Sources
RF	Random Forest
RT	Regression Trees
SoS	System-of-Systems
SP	Stochastic Programming
SRT	Solid Retention Time
SSR	Self-sufficiency Ratio

SVM	Support Vector Machine
SVR	Support Vector Regression
TD3	Twin Delayed Deep Deterministic Policy Gradient
TOU	Time of Use
TST	True Solar Time
TW	Terawatt
TWh	Terawatt hours
UNFCCC	United Nations Framework Convention on Climate Change
URSOFC	Unitized Regenerative Solid Oxide Fuel Cell
USA	United States of America
VBA	Visual Basic for Applications
VMAX	Maximum Volume
VRES	Variable Renewable Energy Sources
WWTP	Wastewater Treatment Plant

List of symbols

C_{annual}^{year-1}	Accumulated annual cash-flow of the previous year
$C_{accumulated}$	Accumulated cash-flow
C_{annual}	Annual cash-flow
N	Day of the year
DS	Daylight savings
η	Efficiency of the system
W_{BUY}	Electrical energy bought by the WWTP (kWh)
W_{REC}	Electrical energy given to the REC (kWh)
W_{L}	Electrical energy load of the WWTP (kWh)
W_{CHP}	Electrical energy produced by the CHP (kWh)

W_{PV}	Electrical energy produced by the PV system (kWh)
W_{SELL}	Electrical energy sold by the WWTP (kWh)
ET	Equation of time
f	factor of conversion
$\dot{Q}_{CHP}$	Flowrate of biogas to the CHP (m^3/h)
$\dot{Q}_{T}$	Flowrate of biogas to the torch (m^3/h)
$\dot{Q}_{B}$	Flowrate of produced biogas (m^3/h)
GHI	Global horizontal irradiance
H	Hour angle
ϕ	Latitude of the geographical location
λ_{local}	Longitude of the geographical location
$\lambda_{timezone}$	Longitude of the time zone
α	Panels tilt angle
PR	Performance ratio
$PV_{production}$	Photovoltaic production
PAI	Plane of array irradiance
$€_{BUY}$	Price of the purchased electrical energy
$€_{SELL}$	Price of the sold electrical energy
SSR	Self-sufficiency ratio
δ_S	Solar declination angle
$\sum$	Sum
$\mathrm{A_p}$	Total area of installed photovoltaic panels
TST_{hours}	True solar time in hours
B	True solar time variable
u	Update rate
$C_{updated}^{year}$	Updated annual cash-flow of the current year

$C_{updated}$	Updated cash-flow
V	Volume of biogas in storage (m^3)
h	Zenith angle

1 Introduction

1.1 Framework

Wastewater treatment plants (WWTP) are one of the primary consumers of energy in modern societies (Daw *et al.*, 2012). These infrastructures are also one of the prime candidates for decentralized production in the industry. The necessity for better management of the energy sources in WWTPs has been widely documented and tackled in numerous studies (Mo and Zhang, 2013; Marcelino *et al.*, 2015; Colacicco and Zacchei, 2020; Odabaş Baş and Aydınalp Köksal, 2022). However, due to the nature of each WWTP, each case is different. The location of the plant, as well as the energy sources at their disposal vary from case to case. Thus, the necessity to further investigate and tackle new case-studies is always paramount.

In this dissertation, an extensive bibliographic review will be undertaken, in order to better understand the current state of the optimization and simulation mechanisms in not only WWTPs, but also in district energy scenarios (Mathiesen *et al.*, 2015; Khorsand and Seifi, 2018; Doubleday *et al.*, 2019), countries (Devlin *et al.*, 2017; Fattahi, Sijm and Faaij, 2020), or singular non-industrial buildings (Foucquier *et al.*, 2013; Theocharides *et al.*, 2018; Ikeda and Nagai, 2021). The same approach will also be performed for the economic analysis, to understand the main methods used for these analysis (Vahid-Ghavidel *et al.*, 2020; Li *et al.*, 2021). Afterwards, a methodology will be developed with the intent of tackling the proposed objectives.

The optimization of energy systems is one of the main ways of achieving cost reduction and minimize the ecological footprint of a WWTP. Allied with economic analysis for potential solutions, a plant will have a strong foundation to build upon and achieve energetic self-sustainability.

1.2 Company identification

This dissertation was done in partnership with SimDouro. The company is responsible for construction, management, and concession of the WWTP system of the *Porto* region, as shown in the map of Figure 1 (*SIMDOURO*, no date). The area of activity of the company is vast, involving the municipalities of *Arouca, Baião, Castelo de Paiva, Cinfães, Paredes, Vila Nova de Gaia,* and a portion of *Penafiel*.

SimDouro provided data and insight on their operations in the WWTP of *Gaia Litoral*. This plant is the main target for the work developed. The WWTP is located in *Vila Nova de Gaia*. The plant possesses two main lines of treatment: a liquid line, where biological treatment occurs inside four biological reactors; and a solid line, where the process of anaerobic digestion and production of biogas takes place. It serves a vast population and has noted an increase in the overall intake of organic matter. This allows for an increase in biogas production, but also an increase in the energetic needs of the WWTP.

In addition to the biogas production, the WWTP will also implement, in the foreseeable future, a photovoltaic (PV) system. This system will bring more stability to the daily operations of the plant, allowing, on paper, to exceed the energetic demands of the plant's, strive for self-sustainability, and cement the plant as productor of renewable energy.

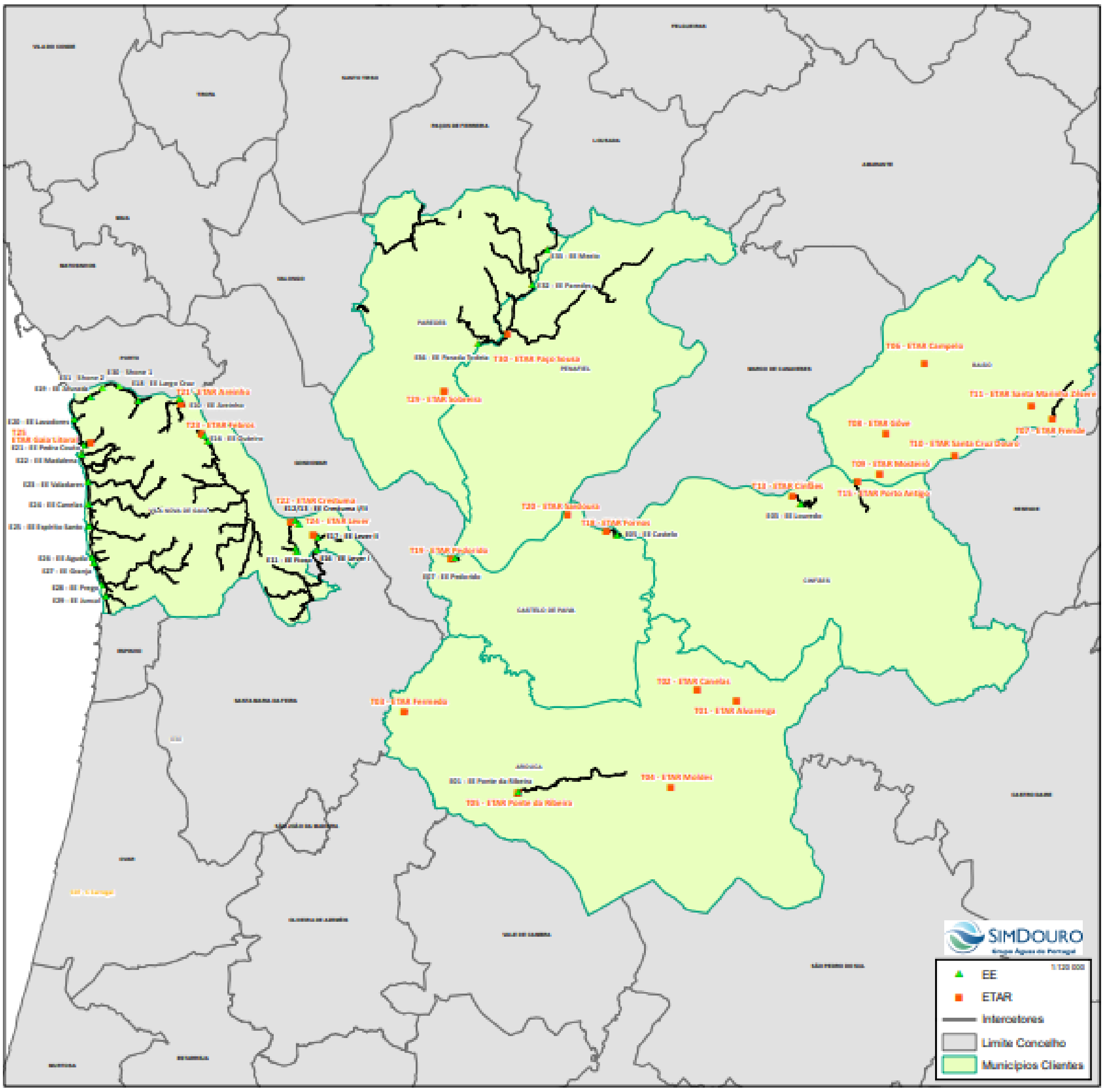


Figure 1 - Map of the area of activity of SimDouro

1.3 Motivation

In times where production of energy is becoming increasingly decentralized, it is fundamental for infrastructures with energy necessities to be able to manage their electricity demands and production. The WWTP is a prime example of an ideal decentralized energy producer/consumer. Not only it has high energy needs but has the possibility to produce energy from a variety of renewable energy sources (RES).

In the specific case of the WWTP of *Gaia Litoral* and SimDouro, it has multiple attributes that make it an attractive prospect for an analysis and for optimization: generates biogas through anaerobic digestion, has a PV installation to take advantage of the solar energy, has potential for expansion and to increase production, and has multiple other infrastructures in close proximity with the WWTP, which makes it an ideal candidate for renewable energy community (REC) implementation (Figure 1). These points combined make this an excellent candidate for testing the possibilities of RES and decentralized production in Portugal and advance the energetic evolution.

1.4 Objectives

The dissertation has two main components: the first one is the creation of an energy optimization system for the WWTP of *Gaia Litoral*; the second is the economic evaluation of investment possibilities for the WWTP.

Understood within the first topic, the main objectives are as follows:

- Minimize the volume of biogas burned in the torch.
- Mitigate the necessity for the WWTP to purchase electricity from the general electrical grid.
- Achieve energetic self-sustainability in the WWTP.

The first two objectives will be tackled with direct approaches, by creating simulation models, while the third objective will be analysed as a byproduct of the first two.

For the second topic, the main objectives are as follows:

- Evaluate the economic benefits of installing the PV system for the WWTP and for other infrastructures belonging to SimDouro.
- Assess the economic impact of installing a second cogeneration of heat and power (CHP) unit, as a way to reduce the amount of biogas burned in the WWTP and produce more energy.

1.5 Structure

The following work is subdivided as follows: chapter two presents an in depth bibliographical review, with emphasis on the topics of wastewater treatment plants, simulators, economic impact, and legislation; chapter three focuses on explaining the fundamentals of solar energy and biogas, as well as recent technological developments in those areas; chapter four details the methodologies used in the project, the followed approaches for optimization and for economic analysis, and the case study that is analysed; chapter five provides the results obtained in this work, along with an individualized analysis for each component; lastly, chapter six presents the conclusions, as well as guidelines for future work development. In Appendix A the literature review of relevant modelling studies is presented in a summary table; in Appendix B it is detailed the VBA code utilized for each simulation, along with basic instructions on how to utilize the code to achieve results.

2 Theoretical background

2.1 Wastewater Treatment Plant

A wastewater treatment plant (WWTP) is a fundamental piece in a civilized society, given that wastewater aggregation is the main cause of water pollution worldwide (Zarasvand Asadi *et al.*, 2013). It is responsible for treating incoming residual water and discharge it to the designated effluents, whilst maintaining water quality inside the legislated limits (Serdarevic and Dzubur, 2019). From the start, the only focus of a WWTP was guaranteeing that these requirements were met successfully, which became increasingly harder with the rise of global population. However, in recent years, and through the approval of energy policies with the objective of increasing reliability, affordability, and sustainability in the energy sector (Fattahi, Sijm and Faaij, 2020), the focus shifted to minimize energy consumption in WWTPs (Moffet, Sirois and Beauvais, 2011), optimize processes (Nakkasunchi *et al.*, 2021), and increase decarbonisation (Berjawi *et al.*, 2021).

WWTPs are one of the main energy consumers worldwide. According to data from Daw *et al.* (2012), it is estimated that 3 to 4% of the United States of America's energy consumption comes from WWTPs. Even though WWTPs function uninterruptedly throughout the entire year, spikes of influent wastewater are noticeable. For instance, has stated by Colacicco and Zacchei (2020), in the Mediterranean area, there are peaks of influent wastewater during the summer, resulting in increased energy consumption. In the economic side, by analysing operating expenses, Odabaş Baş and Aydınalp Köksal (2022) estimated that energy consumption amounted to roughly 25% to 40% of total costs and demonstrated the existence of a positive correlation between total electricity consumption and treated wastewater. Nakkasunchi *et al.* (2021) presented a plethora of factors that influence the overall energy demand of a WWTP such as the presence of nutrient recovery facilities and the number of treatment stages.

Most civil WWTPs provide at least two purification levels: primary and secondary treatment (Colacicco and Zacchei, 2020). Some might have advanced treatment procedures after the two main levels, depending on the effluent quality required by policies and the composition of the water received in the WWTP. Unless it is necessary, this final stage should not be present, since it requires the highest amount of energy (Gu *et al.*, 2017a), followed by secondary and primary treatment, respectively. Each aeration system, responsible for supplying oxygen to the wastewater in the secondary stage, also shows a high auto-consumption (Colacicco and Zacchei, 2020). Sludge treatment, an independent process responsible for compacting and improving sludge stability through all stages, represents 8% of the total energy consumption (Gu *et al.*, 2017a). In an energy audit performed to the largest Italian WWTP, Borzooei *et al.* (2020) showed that the highest fraction of energy uptake is in the aeration process, followed by pumping and operational energy consumption.

Primarily, energy savings can be attained through the application of mathematical models, allowing for a smoother operation throughout the entire facility. With the application of a model-based optimization system, Borzooei *et al.* (2020) was able to achieve 5000 MWh per year in energy savings. Nakkasunchi *et al.* (2021) showed that machine learning (ML) has been used to optimize energy demands in WWTPs. Additional modelling tools have been developed to improve specific processes within the environment. However, the author reiterates that, even after optimization, some WWTPs might remain highly energy-intensive, due to the necessity of maintaining effluent quality in accordance with current policies.

During this century, a new topic of interest has appeared regarding WWTPs: energy sufficiency (Gu *et al.*, 2017b), which can be understood as the ability for a consumer to meet its own demands for energy through the use of self-produced energy. Most commonly, these situations require the implementation of renewable energy sources (RES). Multiple studies (Daw *et al.*, 2012; Cao *et al.*, 2018; Strazzabosco, Kenway and Lant, 2019; Nakkasunchi *et al.*, 2021; Odabaş Baş and Aydınalp Köksal, 2022) have shown that integrating RES in a WWTP can be viable due to their high potential and high energy needs. In some cases, like the ones analysed by Strazzabosco, Kenway and Lant (2019) and Odabaş Baş and Aydınalp Köksal (2022), this integration is only cost-effective if the flow-rate of the WWTP is high enough to justify the use of RES, although lower flow-rates also imply less sludge which results in less energy required for the treatment stages.

Most WWTPs have the resources to implement RES to meet some degree of their own energy demands, as shown in the case of Odabaş Baş and Aydınalp Köksal (2022), which pointed that, in Türkiye, 33% to 55% of energy needs in WWTPs could be fulfilled by RES implemented on site. In order to be self-sufficient, WWTPs must combine multiple RES, as proven in Strazzabosco, Kenway and Lant (2019), in which biogas and photovoltaic (PV) were conjoined for a medium sized WWTP. Odabaş Baş and Aydınalp Köksal (2022) also concluded that an important side-effect of implementing RES in WWTPs is the clear decrease in emissions of greenhouse gases, which may be an incentive to some countries to help WWTPs, in order to meet global objectives, set in the Paris agreement (*The Paris Agreement | UNFCCC*, no date).

The combination of optimization models and RES can be extremely powerful for a WWTP, increasing their system flexibility. According to Devlin *et al.* (2017), system flexibility can be defined as the “overall ability of a power system to respond to changes in demand and online generation”. With the introduction of highly volatile sources of energy, it is mandatory to manage them appropriately to guarantee the maximum efficiency and return of the investment made. Factors such as component degradation, ramp up/down rates, start times, minimum stable generation level, or the ability to give/sell excess energy to the general electrical grid should be taken into consideration to increase the overall system efficiency and flexibility (Cassettari *et al.*, 2017; Devlin *et al.*, 2017), while barriers that hinder progress and inhibit flexibility, e.g. fixed electricity prices, that remove the ability to respond to real-time signals, should be avoided (Møller Sneum, 2021). Above all, the overall quality of the effluent water has to be the number one priority, requiring tight margins and repetitive testing to ensure that water quality remains inside current policies, given that, as presented in the case of Borzooei *et al.* (2020), simple optimizations that are positive for the economic and energy efficiency aspects can cause immediate decrease in water quality.

2.2 Simulators

To be able to optimize the energy needs of a WWTP it is necessary to forecast the energy production and consumption. Attempts to facilitate this process have been made throughout the last 50 years. According to Pfenninger (2017) "Energy system models were first developed in the 1970's by the International Energy Agency (IEA) and the International Institute for Applied Systems Analysis (IIASA)". Since then, massive steps have been taken to advance this area, especially in the last 15 years, with the increase of production of energy through RES, and with the increase in incentives for production-consumers at every level of the society.

2.2.1 Multi-energy systems

With the increasing introduction of RES at the consumer level, more infrastructures are becoming a multi-energy system (MES). A MES involves a holistic consideration of an energy system, covering all the stages, from extraction to treatment and services (Kriechbaum, Scheiber and Kienberger, 2018), while also having the ability to maintain the comfort of the end-users, by relying on numerous energy carriers, increasing the flexibility (ability to respond to external signals in a given time-frame (Møller Sneum, 2021)) within the system (Vahid-Ghavidel *et al.*, 2020). Depending on its characteristics, Mancarella (2014) (cited from Kriechbaum, Scheiber and Kienberger, 2018) concluded that a MES can be categorized according to space, time-resolution, network type, number of services, and number of fuels used. Correctly categorizing a MES is an important step to ensure a good optimization model in the subsequent stages.

For a MES, an energy hub (EH) and an integrated energy system (IES) are two important concepts to define in the context of an energy system management and optimization operation. Although they share some similarities, these two frameworks are non-concurrent and may be used in combination to achieve stronger results.

In literature, multiple definitions can be found for both these concepts. Khorsand and Seifi (2018) defined EH as “a unit that interfaces with consumers, producers, storage devices, electrical transformers, power electronic devices, gas compressors, heat exchangers, or boilers”, while Geidl *et al.* (2007) (cited from Vahid-Ghavidel *et al.*, 2020) defined EH as “a system that has the capability of converting, storing, and managing multiple energy carriers”. Kriechbaum, Scheiber and Kienberger (2018) defined EH as a “generic approach for steady-state modelling and optimization of future interconnected multi-energy networks” while, in the same paper, stated that in IES, “multiple energies are interconnected and converted by various coupling components to satisfy terminal demands”. IES is also defined as the “combined process of acquiring and using energy in a given society or economy” by Jaccard (2006) (cited from Klemm and Vennemann, 2021).

The importance of the application of EH and IES when having to optimize a MES is undeniable (Vahid-Ghavidel *et al.*, 2020). While EH is the interface between participants and transmission system and is responsible for transforming, conditioning, and delivering energy in accordance to consumer needs (Favre-Perrod, 2005), IES focuses on efficiency, reliability, and sustainability by integrating multiple energy sources (Mathiesen *et al.*, 2015; Fan *et al.*, 2021). Cao *et al.* (2018) characterizes IES as reliant on the use of renewable energies, capable of plug and play, and competent at balancing supply and demand through wide-area energy sharing. For IES to be viable, it’s mandatory to implement multiple energy sources (Vahid-Ghavidel *et al.*, 2020). However, at the consumer level, there is a high degree of RES penetration, which can cause an “uncertainty cascade”, as described by Li *et al.* (2021). Li suggests three measures to promote IES independence from the main electrical grid: increase accuracy prediction, modelling RES uncertainties, and stepwise elimination of the adverse influence via multi-stage optimization. Nevertheless, integrating RES in models brings a new set of challenges that need to be taken into consideration such as their rapid deployment, high variability, and the possibility of incorporation of energy storage and grid expansion options in the models, increasing the overall complexity (Kriechbaum, Scheiber and Kienberger, 2018).

The implementation of IES and EH has been widely recorded and studied at the district level, englobing a vast set of buildings and infrastructures in the same optimization scheme (Geidl *et al.*, 2007; Bracco *et al.*, 2014; Powell *et al.*, 2014; Allegrini *et al.*, 2015; Mathiesen *et al.*, 2015; van Beuzekom, Gibescu and Slootweg, 2015; Devlin *et al.*, 2017; Reddy, Sandeep and Jung, 2017; Chen, Alvarado and Hsu, 2018; Khorsand and Seifi, 2018; Kriechbaum, Scheiber and Kienberger, 2018; Doubleday *et al.*, 2019; Chen *et al.*, 2020; Fattahi, Sijm and Faaij, 2020; Ullah *et al.*, 2020; Gao, Li and Hong, 2021; Klemm and Vennemann, 2021; Li *et al.*, 2021; Møller Sneum, 2021; Wang *et al.*, 2021; Jing *et al.*, 2023). However, at the building level, the number of studies is not yet significant, given the particularities that each building possesses, as well as the several different sources of renewable energy (Foucquier *et al.*, 2013; Li and Wen, 2014; Theocharides *et al.*, 2018; Zhang *et al.*, 2018; Ikeda and Nagai, 2021; Mendecka *et al.*, 2021; Gao *et al.*, 2022). With the increase of RES implementation in singular housings, and, most importantly, at the industrial level, the importance of conducting a more in dept approach for this scenario is rising.

2.2.2 Models

Models, as defined by Kriechbaum, Scheiber and Kienberger (2018), are “simplified replicas of the real world systems and may consist of several hard or soft-linked sub-models”. Klemm and Vennemann (2021) stated that "models are an essential tool for planning and operating energy systems; it's a simplified representation of a real world's energy system". Models can be placed in three main categories, according to Chang *et al.* (2021): simulation, optimization, and equilibrium models. The main challenge of creating a model is to accurately model the desired problem, by selecting the adequate factors and boundary conditions. As an example, in the case of Klemm and Vennemann (2021), that intended to model and optimize a MES in a mixed-use district, out of 145 analysed models, only 13 fitted the criteria required for the functions deemed necessary.

The adequacy of a model to the desired problem should be analysed prior to the start. To ensure that the model is appropriate to satisfy the needs imposed by the problem at hands, a few topics should be taken into consideration. Typically, models use one of two approaches, a top-down, for macroeconomic focus, and bottom-up, for techno-economic focus (Kriechbaum, Scheiber and Kienberger, 2018). Models can also be differentiated according to their source code. Models can be open-source or closed-source, meaning that the public can or can't access the code of the model, respectively. Open-source code has the advantage of being easier to manipulate, greater flexibility, increased transparency, better reproducibility, more effective collaboration, and increased productivity (Kriechbaum, Scheiber and Kienberger, 2018). However, developers sometimes prefer to maintain the source code private to preserve sensitive information, due to the amount of time that is necessary to make it open, or even the added bureaucracies that may retard the launching procedures (Kriechbaum, Scheiber and Kienberger, 2018; Klemm and Vennemann, 2021). By deeming that manipulating the code is not an advantageous feature for the model, a greater number of models might be available to select and compare results. Models can also be classified as physical (appropriate for low-complexity scenarios, and high-quality building information is required), statistical (better suited for prediction and optimization; require low information on the building, but high-quality data), or hybrid (good trade-off between both) (Foucquier *et al.*, 2013). Inside the hybrid models, Li and Wen (2014) further subcategorize in white box models (better at capturing building dynamics; more time consuming to develop; more time consuming to solve; requires detailed information and data difficult to obtain; requires expert work), black box models (requires extensive data; large amount of time to train model; easy to build; computationally efficient), and grey box models (hybrid; simplified physical description; simplified physical models; less training data-sets; less calculation time; most common in online building optimal control).

Gao, Li and Hong (2021) compared the costs of different prediction methods at the end of a forecasting week. Results for the analysed models showed that costs vary, depending on the used model, between 11,000 and 11,500 euros. When dealing with a IES, Berjawi *et al.* (2021) encountered new market structures, creation of new interactions, and creation of new interdependencies in the energy system, impacting the structure and function of the model and its overall complexity. In deterministic approaches, uncertainties are neglected, due to planning and scheduling algorithms being relatively simple (Cao *et al.*, 2018), which may create incompatibilities when dealing with a more complex IES system or when highly accurate predictions are required.

Model initializations are an equally important parameter that must be accounted for when planning. Glorot and Bengio (2010) (cited in Díaz–Vico *et al.*, 2017) showed that bad initializations resulted in null centred gradients, affecting the overall results obtained by the model. In Díaz–Vico *et al.* (2017), new forms of activation of DNNs are cited, such as convolutional layers and rectified linear unit (ReLU). Convolutional layers limit the number of hidden layers and avoids the problem of information loss and overfitting, although it only works in restricted spaces, as first submitted by LeCun *et al.* (1998). ReLU, propositioned by Jia *et al.* (2014), has the advantage of accelerated convergence, avoids vanishing gradients, and induces sparsity. Combining sub-models into a singular model can be an effective way to prevent bad initializations and achieve superlative results (Dietterich, 2000; Zhou, 2012).

With the increase of RES implementation in IES, Cao and Lin (2008) deemed fundamental to develop more accurate methods for forecasting the hourly global solar irradiance of the next day and the daily global solar irradiance. Most existing models are based on conventional physical models and statistical assumptions, resulting in a lack of attention to the randomness that is inherent to these predictions, as are examples the models developed by Collares-Pereira and Rabl (1979), Audi and Alsaad (1991), Muneer, Younes and Munawwar (2007), and Jing *et al.* (2023). Empirical models, such as sunshine-based models, which are useful for PV, can also be found in literature (Alzahrani *et al.*, 2017). Powell *et al.* (2014), in a case that intended to predict energetic needs of a university campus with CHP and RES, used meteorological data as an input variable with a high degree of success. Pfenninger (2017) calculated PV production with the global solar energy estimator method. Li and Wen (2014) utilized the following methodology to estimate PV panel power generation: firstly, estimated the total solar irradiance on the tilted surface of the PV panel from overall global solar radiation on the horizontal surface; following that, calculated the absorbed irradiance based on the solar irradiance on the PV cell surface; lastly, computed the PV power generation from absorbed solar irradiance. Bustamante and Liao (2017) attempted to model a solar-biogas hybrid WWTP that could be self-sustainable. The ideal solution obtained consisted of a conjugation of PV, biogas, and biogas storage for short-term energy storage.

Li *et al.* (2021) developed an in-depth study focused on IES with high prominence of RES. RES uncertainties have several ways that can be modelled. Linear programming requires defining an objective function and uses a min-max approach to reach an optimal solution. Although it is easy to implement, it is only appropriate when all system relationships can be described with linear functions. Monte Carlo Simulation (MCS) uses probability density functions (PDF) to calculate objective functions on the basis of input-output relationships and select the best individual at every iteration to achieve an optimal solution (Li *et al.*, 2021). It uses randomness for the solution of problems, by generating random values for uncertain inputs and applying these to simulate a deterministic problem per simulation (Khorsand and Seifi, 2018; Ullah *et al.*, 2020). An increasing number of trials will equal to more accurate results, although higher computational time (Li *et al.*, 2021). MCS is simple and efficient to implement but will generally require superior computational capabilities for convergence, when compared to other algorithms (Khorsand and Seifi, 2018; Ullah *et al.*, 2020). It is mainly used to solve problems with high degree of complexity, nonlinear equations, and due to not requiring additional calculations to function (Khorsand and Seifi, 2018).

Although it may not be useful for every scenario, the use of a rule-based approach to optimize an IES may prove to be an efficient solution. Mendecka *et al.* (2021) utilized this approach. In spite of its simplicity, it's reliable and computationally effective. It consisted of the creation of a flow-chart to establish a control strategy. PV is deemed as the primary source of energy, while the unitized regenerative solid oxide fuel cell (URSOFC) and batteries are secondary. Biogas was also an input flow, produced locally in the anaerobic digestor. To test this approach, commercial buildings in the USA were selected for an off-grid configuration. The buildings belonged to distinct climate zones to account for the variability factors: weather, RES availability, electric load patterns, financial policies, and environmental policies. Three main results were achieved: the optimization target of 100% RES without excess energy is only achieved if the digester produces from 6000 stdm^3/y to 9500 stdm^3/y, depending on the climate zone; reference configuration allows for the non-use of internal combustion engine, while minimizing (often to zero) the waste of excess energy; by reducing biogas availability or starting with a low state of charge, the use of diesel generator cannot be avoided. Due to the nature of solar energy, PV is traditionally considered as the primary source of energy and given priority. In spite of being easy to implement, this strategy will often stride away from the optimal solution for the problem in hands (Li and Wen, 2014).

On the review made by Fan *et al.* (2021), the most commonly used methods to deal with uncertainties when solving an IES model were robust and stochastic programming. Robust optimization uses intervals to model uncertain variables and does not need accurate probability distribution functions and fuzzy membership functions (Cao *et al.*, 2018). It is used when "the probability of a random variable is unknown, but its fluctuation range is known. The optimal solution is less susceptible to changes in the parameters", has retrieved from Fan *et al.* (2021). According to Li *et al.* (2021), robust programming leads to a conservative solution even when an attempt to combine it with other methods is made. Lu *et al.* (2019) (cited in Li *et al.*, 2021) proved that robust optimization is too conservative for certain scenarios. Fan *et al.* (2021) states that stochastic programming (SP) "involves adding random variables into the mathematical model while considering the probability distribution and correlation of the random variables in the modelling”. Following the same review made by Fan, SP is divided into three main methods: expectancy method, which replaces the value of a random variable with the expected value for said variable, leading to large errors; chance constraint uses PDF of uncertain variables, with its main drawback being that it is difficult to obtain a solution; and multi-scenario, which samples the uncertain factors and creates boundary conditions through the use of a large dataset. According to Li, SP is usually adopted in the prediction of RES. Stochastic considers multiple uncertainty parameters at the same time and particularly useful in the optimization of IES at a small scale, with combination and integration of the general electrical grid (Kuznia *et al.*, 2013; Reddy, Sandeep and Jung, 2017). Even though it is harder to escalate, it is more efficient than MCS (Li *et al.*, 2021). Some parts of an IES, such as the behaviour and charging patterns of electric vehicles, have an almost completely stochastic configuration, making the use of traditional and simpler methods impossible and requiring the use of stochastic programming to model it (Strezoski and Stefani, 2021). In Cao *et al.* (2018), chance-constrained programming and two-stage stochastic programming were used to handle multi-objective economic load dispatch, by using a jointly distributed random variables method. In Li *et al.* (2021), a three stage multi-stage optimization strategy is presented. The first stage is a day-ahead dispatch, the second stage consists of intra-day scheduling, and the third stage is real-time control. According to the literature research, this methodology has not yet been implemented in a WWTP situation. However, it is a valid alternative, since it will generate a prediction with a day of spare time, then it will verify said prediction on the same day with fresh data, and will, in real-time, make sure that no unexpected fluctuations will put the safety of the IES at risk.

According to Li *et al.* (2021), artificial intelligence (AI) has shown that it can be a valuable tool to increase forecasting accuracy. AI takes advantage of its strong data mining ability in order to directly generate uncertain scenarios with actual data instead of fitted PDF. It is more advanced, complex, fault-tolerant, can work with noisy or incomplete data, faster than conventional algorithms, and can contribute to a deeper understanding of the system (Ahmad, Zhang and Yan, 2020; Klemm and Vennemann, 2021). In order for AI to be viable, prediction accuracy must remain at a high standard, otherwise its viability is compromised (Ikeda and Nagai, 2021). The branch of AI focused on developing algorithms and models is machine learning (ML) (Lv and Tang, 2011; Sarker, 2021).

An artificial neural network (ANN), according to Theocharides *et al.* (2018), “constructs relationships between a set of input features and the output using a model derived from our understanding of how a biological brain responds to stimuli from sensory inputs". As stated by Cao and Lin (2008), ANN models have been applied to forecasting solar irradiation and found more accurate results than the conventional models. Despite being more versatile and achieving more accurate results, there are some downsides to the use of ANN. Ehlhardt *et al.* (2023) stated that the two-step approach is not applicable when ANNs are used as the

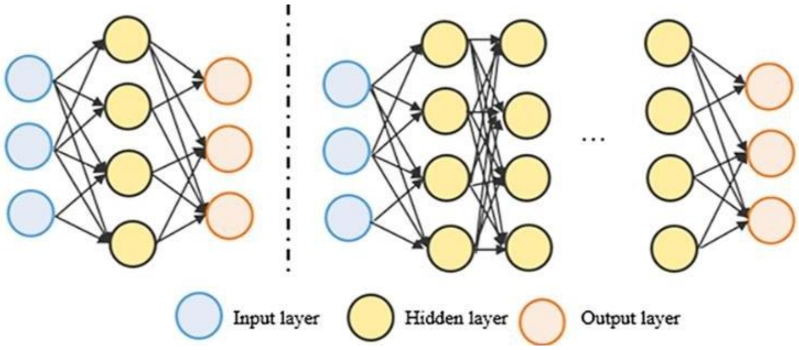


Figure 2 – Comparison between an ANN (on the left) and a DNN (on the right). Adapted from Hernandez Martinez, Ariza and Castillo (2020)

optimization model, due to the large number of parameters without physical meaning, contrary to Cao *et al.* (2018), where two-stage stochastic programming was a viable possibility to achieve solid results. While an ANN only possesses a singular hidden layer between their input and output layer, deep neural networks (DNN) “can be defined as ANNs with several hidden layers” (Díaz–Vico *et al.*, 2017), has illustrated in Figure 2. Ahmad, Zhang and Yan (2020) reviewed existing studies for prediction models with effective RES management. There was a clear focus on efficiency, stability, and performance of the predictions, making ML, ANN, and ensemble-based approaches the best and most frequent solutions.

In Appendix A (page 77) it is presented a comprehensive review of existing relevant studies for models applied to IES and EH. As it can be analysed, there are plenty of other models used in literature, in addition to the already mentioned. For use in PV forecasting, Theocharides *et al.* (2018) considers the persistence model (PM) as the simplest type that can be used to achieve solid results. PM is "a data structure algorithm that preserves its previous version when it is reformed”, with its main downside being that it assumes that the conditions will not suffer any changes in the foreseeable future. Regression trees (RT) is a method that “recursively partitions the data to a simple prediction model within a partition of the split data, using the analysis of variance method in order to analyse the differences or variations among the data partitions" (Theocharides *et al.*, 2018). It doesn’t require data normalization or data scaling and its able to model non-linear relationships, although it can lead to overfitting and have low model stability (Lai *et al.*, 2020; Zagajewski *et al.*, 2021). Support vector machines (SVM) “use multidimensional surfaces to define the relationship between features and outcomes" (Theocharides *et al.*, 2018). They are computational complex and hard to interpret, but are also very robust and flexible, which are valuable resources for modelling an IES (Lai *et al.*, 2020; Montesinos López, Montesinos López and Crossa, 2022; Sarang, 2023). Selecting a model appropriate to the necessities of the IES is fundamental to guaranteeing accurate results in the most efficient way possible.

2.2.3 Pre-processing

Motivated by the increase in RES penetration at the consumer level, studies have been conducted to assess the impact in different models of uncertainty level (Chae and Kang, 2013; Díaz–Vico *et al.*, 2017; Cao *et al.*, 2018; Borzooei *et al.*, 2020; Guevara *et al.*, 2020; Gao, Li and Hong, 2021; Ikeda and Nagai, 2021), assumptions (Borzooei *et al.*, 2020), variable sensitivity (Chae and Kang, 2013; Laayati *et al.*, 2022; Jalving *et al.*, 2023), and constraints (Cao *et al.*, 2018). The impact caused by shifts in each parameter was usually evaluated through the required computational time (Moffet, Sirois and Beauvais, 2011; Khorsand and Seifi, 2018; Mylonas *et al.*, 2020), the data required for the model to function (Alzahrani *et al.*, 2017; Theocharides *et al.*, 2018; Borzooei *et al.*, 2019; Strazzabosco, Kenway and Lant, 2019; Gao *et al.*, 2022; Odabaş Baş and Aydınalp Köksal, 2022), or achieving predetermined objectives (Cao *et al.*, 2018; Vahid-Ghavidel *et al.*, 2020; Gao *et al.*, 2022).

Li *et al.* (2021) reiterated the importance of establishing objectives prior to the creation of the model to guide the progress when used to optimize an IES. These can be economic (cost reduction, benefit improvement, lowering purchasing costs, or lowering operating costs), environmental (lowering the excess carbon or greenhouse gas emissions), or energy saving objectives in the various phases (generation, consumption, or utilization efficiency). By expressing the desired system behaviour in an objective function and then optimizing said function, the modeller will achieve the best possible results in a direct way (Li and Wen, 2014). Gao *et al.* (2022), in a hybrid system combining photovoltaic (PV), storage, and traditional equipment, defined their optimization target has gradually achieving off-grid operation, by ensuring that the hourly power purchase from the grid is stable in a small range. Vahid-Ghavidel *et al.* (2020) stated, after reviewing demand response programs in MES, that the most common approach used when modelling is to maximize benefits and minimize costs. This has been corroborated by several different authors, who also adopted a cost minimization approach in their models, establishing the minimization of life cycle cost or net present value (NPV) as their main objective (Piacentino *et al.*, 2013; Bracco *et al.*, 2014; Pfenninger, 2017; Bao *et al.*, 2019; Chen *et al.*, 2020). Similarly, in Cao *et al.* (2018) review, the most commonly used objectives when optimizing were the maximization of capital benefits, maximization of energy benefits, and minimization of losses in natural gas. When comparing multiple models, the use of indicators, selected beforehand to compare their performance, such as the key performance indicator (KPI), is shown by Chae and Kang (2013) and Cassettari *et al.* (2017) to be an effective strategy.

As demonstrated in the chapter 2.2.2, when optimizing, multiple types of models can be used. When reviewing the existing literature, three main reasons are appointed as to why advanced models that use ML or ANN must be employed: model uncertainty, number of variables, and computational time. Guevara *et al.* (2020) justified the use of mixed-integer linear programming (MILP) with the 240 parameters of uncertainty associated with the model. Ikeda and Nagai (2021) had a total of 168 variables, resulting in 21168 possible combinations, which was deemed unsuitable for linear programming. When using DNN to predict the total daily incoming solar radiation in a region of Spain, Díaz–Vico *et al.* (2017) had a total of 10800 different inputs, resulting in 4380 training patterns.

In the cases presented previously, the use of any form of ML was required due to the high number of variables. However, it is also important to reduce the computation time to the minimum possible, especially when the main objective is to forecast and optimize in real-time (Mylonas *et al.*, 2020). As such, ML may be used with the intent to diminish the computational burden carried by using simpler programming. Perera *et al.* (2019), with hybrid optimization algorithms, managed to reduce computational time by 84%. The reduction of computational time is not limited to the type of programming used, as shown in Mylonas *et al.* (2020), where different hardware was tested and a thirty minute time save per simulation was achieved. Another common way to achieve results in smaller time frames is by reducing the number of variables and iterations. The total number of variables and iterations should be the strictly necessary to achieve solid results. Khorsand and Seifi (2018) demonstrated, in a Monte Carlo simulation (MCS), that 5000 iterations was the ideal number of iterations and, after that point, only an increase in computational time was registered and Moffet, Sirois and Beauvais (2011) showed that calculation time increases linearly with the number of elements in a model. In order to determine which variables and inputs can be removed, simulations can be executed to perceive and compare the sensitivity of the model to some variables. Jalving *et al.* (2023), in a IES optimization framework determined that generator revenue and capacity factor were sensitive to every parameter studied, with marginal cost being the most important factor, followed by startup cost and no-load cost. Chae and Kang (2013), in a small WWTP in South Korea with PV and hydropower, concluded that thermal energy recovery was the most influential factor for the model.

Pfenninger (2017) focused on analysing the impact of different techniques to reduce the time resolution, whilst assessing their accuracy. It was just has important to determine ways to reduce time resolution in the most efficient way possible, as it was maintaining scientific accuracy. Results were not promising, given that they showed significant seasonal and inter-annual variability, meaning that one year may not be representative of others. Bao *et al.* (2019) used inter-hour to focus on optimizing outputs of CHPs and flow rate at gas source node, while intra-hour was reserved for the mitigation of uncertainties, given that RES's persistent prediction errors will have a significant impact on the operation in the long term. Results demonstrated the necessity to consider gas transmission dynamics both in intra-hour and inter-hour, through the active comparison with a steady-state model. Ringkjøb, Haugan and Solbrekke (2018) also separated the objectives for each timeframe, with hourly timeframe focused on making sure that the energetic needs are being met and give a destination to excess energy, while the longer timescales are used to identify pathways to a renewable and emission free energy system. Although increasing the time horizon can be advantageous and, sometimes, required, unnecessarily large horizons will affect the precision of the shorter time splits (Cuisinier *et al.*, 2021). Temporal resolution is impacted by data availability, time-step, coverage, maximum computational time, precision required, and level of description desired for the model to have (Després *et al.*, 2015). The time step for the model is also an important point to define. van Beuzekom, Gibescu and Slootweg (2015) (cited in Kriechbaum, Scheiber and Kienberger, 2018) suggested, for an IES with RES implementation, a 15 minute time-step as adequate.

ML algorithms require an extensive dataset, as seen in chapter 2.2.2. Prior to the development of the model, it is fundamental to gather the important data for the model to function, being heavily dependent of the sources of energy existent in the MES. Kriechbaum, Scheiber and Kienberger (2018) exposes the most common challenges, that include data availability, data quality, and increased model complexity. Kriechbaum also explains that data usually carries their very own set of problems, in addition to the aforementioned issues, such as not being measured, commercially confidential, future related, highly uncertain, or of doubtful quality, affecting the capabilities of the model to generate accurate predictions. Gao *et al.* (2022) retrieved dataset which includes 15 months of hourly data, with features of holidays, hour of the day, power demand, maximum power generated by solar irradiation, and solar irradiation for a hybrid system combining PV and storage. Laayati *et al.* (2022) created a database, which can be used to retrieve data, choose a goal, select inputs and outputs, and finally compare the prediction of different algorithms. Cao and Lin (2008) used a data set of nine years and only a single year as a training set. Also, in an attempt to reduce randomness, the average value of seven successive records takes the place of the central one in the new series. Alzahrani *et al.* (2017) retrieved data on irradiance values on the desired location over four separate days with different cloud coverage. Data was treated, by replacing misread values and the ones that exceed the theoretical limit with either an interpolation of the adjacent values or the theoretical limit itself. Solar irradiance at night was also eliminated for the sake of simplicity, enhance performance, and reduce computational time. All of the existing data was normalized, scaling it between zero and one, and split into three sets: 70% for training, 15% for testing, and 15% for validation. Theocharides *et al.* (2018), in his ML algorithm for PV prediction, also divided the data into the same splits, with the difference that, in a first approach, data was taken successively, whilst in the second approach, data was organized at random. Odabaş Baş and Aydınalp Köksal (2022), when analysing 240 WWTPs in Türkiye filtered the dataset and determined that 10% of the WWTPs were outliers.

At the time of Cao and Lin (2008), cloud cover had not been successfully implemented in ANN model for irradiation forecasts. This was due to the fact that some data also requires interpretation and the creation of a scale that allows for it to be introduced in a mathematical model, a method now called defuzzification or fuzzy analysis. When dealing with weather forecasting, Cao and Lin (2008) used defuzzification for cloud cover data, implementing a scale from 0 (clear sky) to 10 (storm weather). Fuzzy analysis has been widely used to deal with insufficient data and uncertain load demand (Cao *et al.*, 2018).

Gao *et al.* (2022) affirmed the importance of creating a balance between the need to explore the environment and the fact over exploring can affect the convergence speed of the algorithm, especially when dealing with small timeframes. Alzahrani *et al.* (2017) determined that a dataset of solar irradiance is an obligatory step in order to create a functioning PV model. The use of solar irradiance datasets by various authors in their models corroborates this statement, whilst also collecting data of historical solar PV production (Cao and Lin, 2008; Theocharides *et al.*, 2018; Strazzabosco, Kenway and Lant, 2019; Colacicco and Zacchei, 2020; Odabaş Baş and Aydınalp Köksal, 2022). Notwithstanding the data collected, Gao, Li and Hong (2021) still achieved relatively large prediction errors for PV, due to high variability, requiring further investigation and evaluation of variable and data sensitivity, to mitigate the persisting high error. To forecast biogas production, it is important to retrieve historical production and consumption of biogas data, as well as energy produced through combined heat and power (CHP) (Strazzabosco, Kenway and Lant, 2019; Odabaş Baş and Aydınalp Köksal, 2022). Lastly, collecting data of the electricity demand of the WWTP is fundamental to achieve a functional model (Borzooei *et al.*, 2019; Strazzabosco, Kenway and Lant, 2019; Odabaş Baş and Aydınalp Köksal, 2022).

2.2.4 Modelling tools and software

Modelling tools were defined by Chang *et al.* (2021) as “computational software, or modelling frameworks, that generate energy system models”. Klemm and Vennemann (2021) differentiated between model generators and model frameworks, stating that the first one are tools that can create models, although it comes at the expense of low flexibility; whilst the second one are structured toolboxes that include several model generators inside itself.

Chang *et al.* (2021) developed an in-depth compilation and review of 42 review articles that focused on the topic of modelling tools. It was complemented by questionnaires, directly sent to developers and key users of these tools, allowing for a greater understanding of their capabilities. Overall, 54 modelling tools were analysed. In a cited review, Connolly *et al.* (2010) only found seven energy systems modelling tools that were capable of modelling 100% RES systems. Models, in general, were poorly prepared for RES at this time. In order to model variable RES, the model is obliged to have a high level of detail in the temporal, technical, and spatial fronts (Collins *et al.*, 2017). Otherwise, if a low level of detail is used, it will result in low number of averaged time-slices and crude representation of electricity (overly restricts the deployment of VRES; overestimates or underestimates the cost of GHG). It’s impossible to create a modelling tool that encompasses all the desired methodologies, forcing the need for compromises and adaptations. Additionally, due to their in-house development, some tools have virtually no use outside the realm of academia, making it harder to develop for industrial or everyday use. Cross-platform can be used to mitigate some of the aforementioned issues, although most tools don't support as a default capability. Instead, users resort to soft-linking modelling tools: there's no interlinking of source-code between two tools (hard-linking), instead, the inputs and outputs from different tools are connected to achieve better results. If two tools generate a brand new one, by intertwining their code, the new tool can be considered fully integrated.

Time is also an important factor to consider. Chang's review found that the most common time-step among modelling tools is one hour. High temporal resolutions are better able to capture system loads and renewable energy generation, with the downside of being computationally expensive. Poncelet *et al.* (2016) is cited for his study, which concluded, on the topic of temporal resolution in RES, that low temporal RES can underestimate operational costs and overestimate generation capacity. Time horizon is also important to consider, since a lower time horizon results in a smaller computational burden and less uncertainty. However, the time horizon must be adequate to the desired outputs.

Groissböck (2019) analysed 31 modelling tools. Out of those, 11 used Python as their programming language. Those were also the ones that were the most effective in short, long, and mixed term. The remaining tools mostly used GAMS, AMPL, or AIMMS, due to the fact that they allow for easy exchange functions, functionality, and ideas between the different modelling approaches. The exception to these were the modelling tools that worked via executables. These allow for easier control for the user but come at a cost of harder flexibility and removes capabilities for the user to personalize the model.

The field for modelling tools and software that can be used to generate forecasts is vast. The selection is heavily dependent on the necessities of the user and characteristics of the energy system. To extract climate data for the city of Suwon, to be used as input parameter in their model for a WWTP, Chae and Kang (2013) used the RETScreen software. Moffet, Sirois and Beauvais (2011) reviewed three tools: GridLAB-D, OpenDSS, and APREM for a long-term simulation. Findings showed identical results for each scenario, with the main differences appearing in the electrical results. Additionally, OpenDSS was tested for when it was run directly and through MATLAB. The results showed that OpenDSS is faster if executed directly instead of running through MATLAB. Laayati *et al.* (2022) used MATLAB to create their model for educational purposes. Piacentino *et al.* (2013) developed the optimization code in the MATLAB-LINDO hybrid environment. Groissböck (2019), after comparing and examining 31 modelling tools, concluded that the preferred open-source modelling tools were Switch, TEMOA, OSeMOSYS, and pyPSA. These tools considered details such as multi-year investment, year-varying capital and operational costs, and budget and emission constraints. Allegrini *et al.* (2015) reviewed modelling tools for district scale. It was determined that there were two main ways to model solar radiation on an urban scale: through raster digital elevation models, with the advantage of being readily available, although only being 2.5D; or vector computer-aided design (CAD), which is time consuming and expensive. In addition, EnergyPlus, ESP-r, and IDA ICE were determined to be the best building level modelling tools, whilst HOMER, EnergyPro, and RETScreen were selected as the best for RES. Ringkjøb, Haugan and Solbrekke (2018) reviewed 75 modelling tools that had been used in literature for energy and electricity system analysis.

Díaz–Vico *et al.* (2017) highlighted new software's on the rise with high computational capabilities: Caffe, Pylearn2-Theano, Google's TensorFlow, and Keras. Kriechbaum, Scheiber and Kienberger (2018), during the review open-source modelling frameworks, mentioned three main tools that had proven to be useful: Calliope, useful for a large number of scenarios, written in Python, and with a clear separation of framework and model; open energy modelling framework (oemof), with a superior ability to adapt, flexible time resolution, and connection to multiple regions and sectors; and urbs, especially focused on optimizing storage and minimizing costs in energy systems. Calliope was also used by Pfenninger (2017), combined with renewables.ninja to provide high resolution data (both in the temporal and the spatial fronts) of the United Kingdom, for PV and wind. For power representation, Després *et al.* (2015) focused on PRIMES, Switch, REEDS, E2M2, and ELMOD modelling tools, since these had, at the time, the best capabilities.

In their techno-economical evaluation of 456 urban WWTPs in Türkiye, Odabaş Baş and Aydınalp Köksal (2022) utilized HOMER, a simulation program developed by the National Renewable Energy Laboratory (NREL). It optimizes the hourly performance of the various system components for minimum NPV, based on the predefined technical constraints and parameters. The simulated system consisted of a biogas generator, a group of PV modules, and an inverter. It was also connected to the grid to meet electricity demands and sell electricity. Simulation program is feasible and can predict electricity consumption and production with an average absolute error margin of 4.88%. Kasaeian *et al.* (2019) utilized HOMER to model biogas and PV in a hybrid facility. Halaby, Ghoneim and Helal (2017) also used HOMER to model RES potential, among other aspects. Through this modelling tool, it was possible to determine the optimum size of each subsystem present, with the objective of minimizing life cycle costs or NPV. Similarly, Helal, Ghoneim and Halaby (2013) utilized HOMER to model PV and wind in their study for a self-sustained WWTP.

As can be seen through the presented literature, there's a plethora of modelling tools and software's that can be used to model, optimize, and assist in daily decision making. However, it is important to select the correct tool that satisfies the necessities of the problem in hands. A thorough analysis of the ideal characteristics which the modelling tool should have is mandatory. Since each software is different, there might not exist a tool that satisfies all of these features. Due to this, an hierarchisation of these attributes can be necessary to decide between software and achieve the maximum potential for optimization and energy efficiency.

2.3 Economic impact

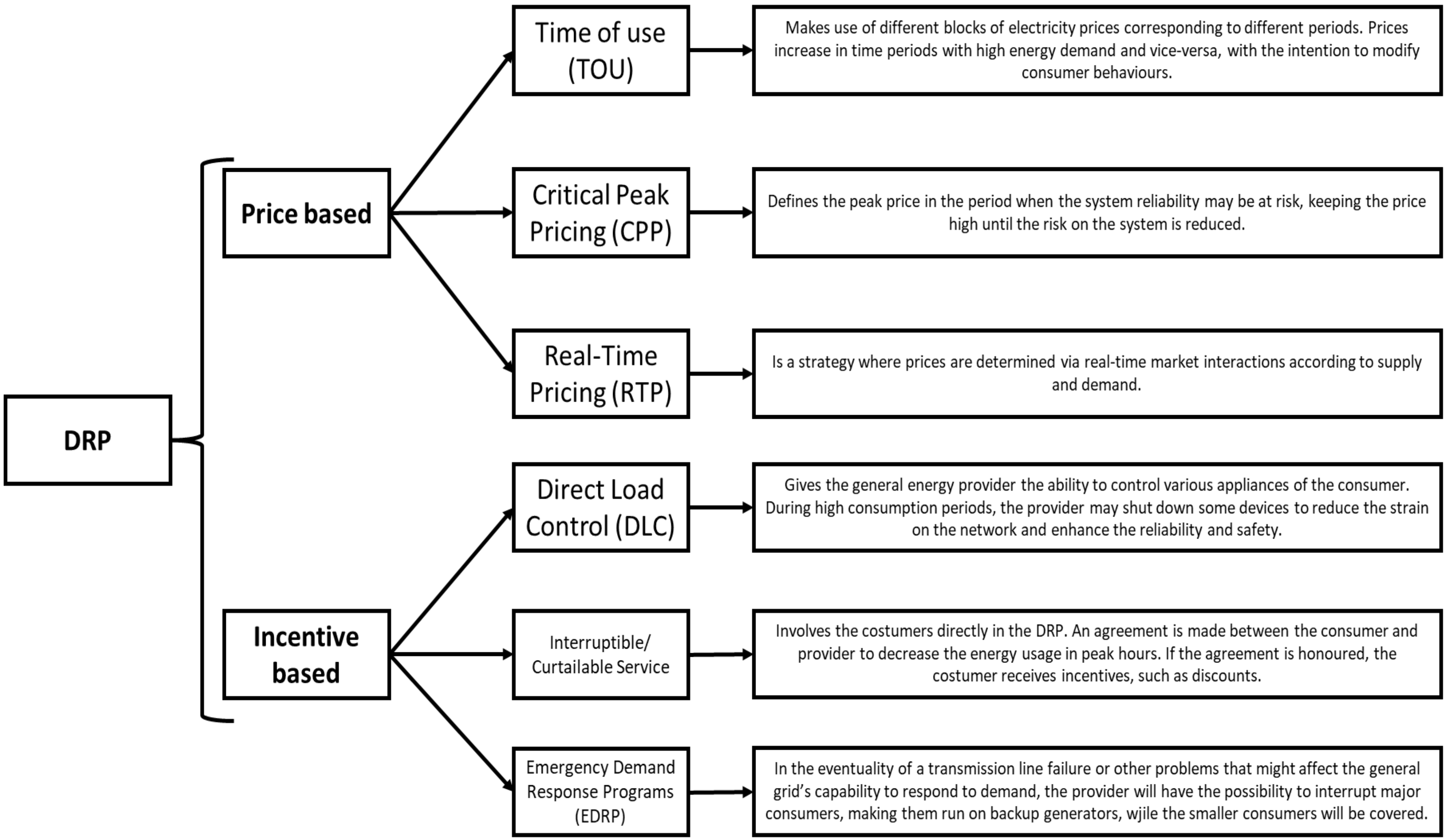
In order to minimize costs, one of the main factors to take into consideration is energy market and its prices (Li *et al.*, 2021). Even if the ultimate goal is to have a self-sustainable project, that may not be possible during the entire day. Market environment plays an essential role in the operational decisions. Energy companies can change prices and time periods to motivate consumers to adjust their consumption to the production (Li *et al.*, 2021). This represents an important challenge for the current energy system, due to the ongoing mass electrification of our society (Vahid-Ghavidel *et al.*, 2020).

Vahid-Ghavidel *et al.* (2020) elaborates on this issue. Demand response programs (DRP) have the goal to manage load profiles through elasticity peak shaving and valley filling. Results can be brought about by the use of time-dependent tariffs, even though it's not always enough to convince a costumer to participate in DRP. In price-based DRPs, the main tool used to modify consumer habits is fluctuation in electricity prices. In incentive-based DRPs, the main trigger to change consumer habits is the offering of rewards. Figure 3 presents a schematic representation of some of the main DRP, as well as a definition for each.

As seen in section 2.2.3, before designing a model, it is important to establish objectives. Commonly, these objectives are economic (Chae and Kang, 2013; Piacentino *et al.*, 2013; Bracco *et al.*, 2014; Cassettari *et al.*, 2017; Pfenninger, 2017; Cao *et al.*, 2018; Bao *et al.*, 2019; Chen *et al.*, 2020). Thus, to evaluate the results obtained by the model, it becomes important to do an economic analysis of the results. This can be made through, feasibility studies (Xu *et al.*, 2017; Kasaeian *et al.*, 2019), sensitivity analysis (Halaby, Ghoneim and Helal, 2017; Kasaeian *et al.*, 2019; Mendecka *et al.*, 2021), or by calculating economic indicators (Foley, 2010; Helal, Ghoneim and Halaby, 2013; Taha and Al-Sa'ed, 2017; Kasaeian *et al.*, 2019).

In Kasaeian *et al.* (2019), a feasibility study was conducted with the intention of verifying if the model was making the hybrid production unit provide reliable energy at the minimum possible cost. The effects of economic conditions and governmental policies (inflation rate, discount rate, subsidies, among others) on system costs and the overall performance were analysed. The unit utilized PV, diesel, and biogas to produce energy, and batteries were excluded due to their high cost of purchasing. Economic indicators, such as NPV, capital recovery factor, cost of energy, interest rates, operating costs, and emission penalties were calculated. Results showed the importance of government subsidies and facilities to facilitate the decision of installing PV; biomass, as a power source, had low efficiency and was not cost effective; the price of diesel does not have a large effect on the economic parameters; discount rates and a higher initial capital can increase the economic benefits exponentially in a medium-long term; and an increase in interest rates makes has a substantial toll on the overall profits margin. Xu *et al.* (2017) intended to explore the influence of the policy side over the WWTP structure. For that, it was used scenario analysis, allowing for an investigation of the feasibility of energy self-sufficiency in the WWTP. The study was based on a WWTP in China. Four scenarios were analysed: baseline, energy reduction, energy reuse, and combined. Results showed that it is possible to achieve self-sufficiency in WWTPs through energy saving and RES production (CHP and PV).

According to Halaby, Ghoneim and Helal (2017), a sensitivity analysis “helps assess the effects of uncertainty or changes in the variables over which the designer has no control". In this study, the main objective was the lowest possible NPV. Three sensitivity cases were tested: the effect of individual RES potential on system NPV; the effect of varying all RES on optimal system type; and the effect of capital costs variation on power. Due to existing fuel limitations, the size of CHP was not subjected to any variation. Results showed that a change of solar



Makes use of different blocks of electricity prices corresponding to different periods. Prices increase in time periods with high energy demand and vice-versa, with the intention to modify consumer behaviours.

Defines the peak price in the period when the system reliability may be at risk, keeping the price high until the risk on the system is reduced.

Is a strategy where prices are determined via real-time market interactions according to supply and demand.

Gives the general energy provider the ability to control various appliances of the consumer. During high consumption periods, the provider may shut down some devices to reduce the strain on the network and enhance the reliability and safety.

Involves the costumers directly in the DRP. An agreement is made between the consumer and provider to decrease the energy usage in peak hours. If the agreement is honoured, the costumer receives incentives, such as discounts.

In the eventuality of a transmission line failure or other problems that might affect the general grid's capability to respond to demand, the provider will have the possibility to interrupt major consumers, making them run on backup generators, wjile the smaller consumers will be covered.

Figure 3 - Main DRP (adapted from Vahid-Ghavidel et al. (2020))

radiation resulted in a total NPV almost constant; lack of anaerobic digestion resulted in high NPV, due to the increased necessity of installing high amounts of batteries, PV, and wind to maintain sustainability; if CHP input flow increased, it would result in a drop in NPV; maximum CHP size should always be considered, given that its capital cost doesn't affect size selection; and that achieving sustainability in a WWTP is possible in rural areas, and even economic in some cases. Mendecka *et al.* (2021) performed a sensitivity analysis on biogas production rate, battery state of charge, and different geographical contexts.

Helal, Ghoneim and Halaby (2013) analysed a case study of a WWTP in Toukh, Egypt. The objective was to evaluate the economic feasibility of using biogas in addition with other intermittent RES, such as PV, in a small-scale rural WWTP. Ultimately, it was intended to achieve self-sustainability and low emissions. The optimal solution should be a system that satisfies the user defined constraints at the lowest life cycle cost or NPV. 16 scenarios were tested. In the end, to achieve self-sustainability, the WWTP would require working at full CHP capacity, 200 kW wind turbine, 100 kW PV, 720 batteries, and 80 kW converter. In the analysis, biogas was found to be more economic than PV or wind technologies. The batteries were the most expensive component, but were necessary for nighttime, especially since this is an islanded IES, which should be self-sufficient. Taha and Al-Sa’ed (2017) studied three different cases of WWTPs. PV off-grid had a payback of eight years, and applications for RES were found on all, especially during emergency situations. Foley (2010) performed an economic analysis for PV installation. It was deemed that the installation can be viable, depending on current policies and energetic needs of the WWTP. Furthermore, it confirmed that a WWTP can become self-sufficient with the current technologies.

2.4 Legislation

In the last decade, there has been an exponential increase in decentralization of energy production through the use of RES. Centralized systems, due to current policies, are more beneficial and reliable (Kasaeian *et al.*, 2019). In the current state, it does not require supplementary bureaucracy, a substantial initial investment, nor to install additional equipment. However, that comes at a cost of a loss of flexibility, lower energy efficiency, and possibly more environmental damage. With the advancement of technology, decentralization is becoming a more prominent and viable alternative. Decentralized systems don't need a lot of additional equipment nor land, are usually installed close or even inside the end-user facilities, have minimized transmission losses, and are simple to maintain (Mehleri *et al.*, 2012, cited in Bracco *et al.*, 2014; Kasaeian *et al.*, 2019). This reality forced the governments to create new legislation to regulate self-producers and self-consumers.

Policy and laws are one of the largest factors and contributors towards greenhouse gas (GHG) emissions reduction (Devlin *et al.*, 2017) and, citing Wang *et al.* (2019), "existing studies rarely consider the environmental impacts of carbon trading on the networks operation". Only a fraction considers carbon emissions, and that is also visible in the existing models, given that only a selected few are capable of mimicking and simulate these factors, as seen in section 2.2.4. Masłoń *et al.* (2020) focused on improving efficiency and reducing emissions in a WWTP. The WWTP had three CHPs, with an average production of 2.54 GWh/year. There was, however, monthly fluctuation. Autumn months were the highest production months. Through optimization, and utilizing data from the previous three years, it was possible to reduce overall emissions of CO_2. CHPs covered from 93.0% to 99.8% of the electricity of the WWTP, resulting in 98.2% self-sufficiency level. Additionally, compared to the use of conventional fuels, the operational costs were reduced and there was less emission of pollutants. Through the use of models for optimization, energy efficiency, economic savings, and environmental benefits can be exponentially increased.

2.4.1 In Portugal

According to data from the European Union (2023), GHG emissions in Portugal, in 2022, were 57.2 $MtCO_2$-eq, which represented an increase of 1.2% in comparison to the previous year. Portugal continues to be ahead of the EU average in terms of GHG domestic emissions, as shown in the graph of Figure 4.

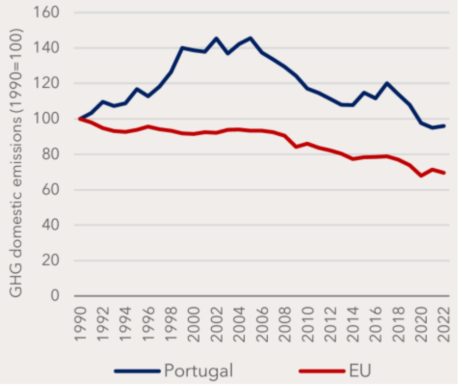


Figure 4 - Comparison of GHG emissions between Portugal and the EU, since 1990 (adapted from (European Union, 2023))

Internally, Portugal's energy sector is the main responsible for GHG emissions, as seen in Figure 5. In the residues and waste sector, there was an increase of its share of GHG emissions when compared to 2020, from 7.6% to 10.0% (*Emissões setoriais de CO2eq., em Portugal, em 2022 | Relatório do Estado do Ambiente*, no date; *Emissões GEE | Agência Portuguesa do Ambiente*, no date). However, the overall emissions have declined in the past years with the increased use of biogas in WWTP.

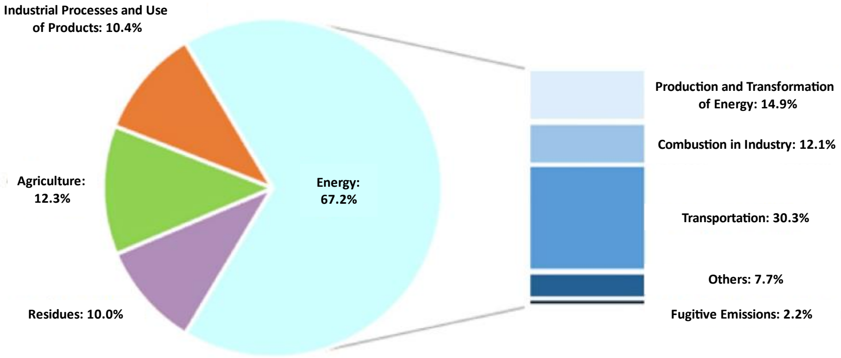
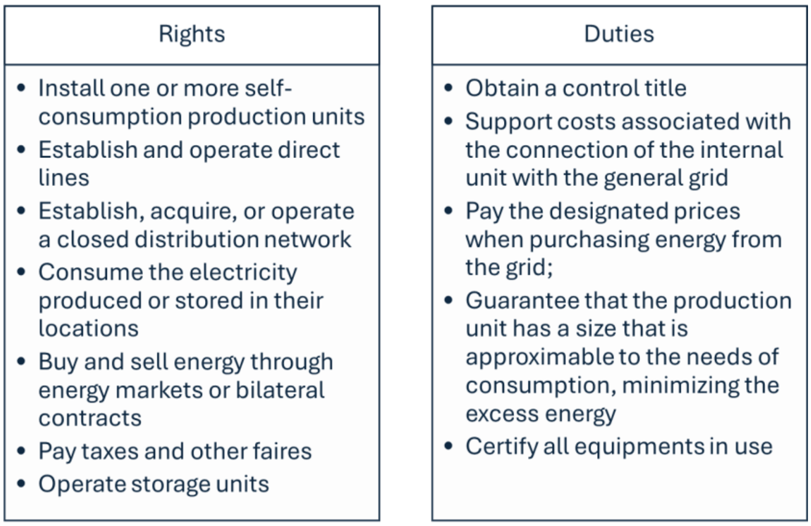


Figure 5 - Sectorial emissions of CO_2-eq, Portugal, 2022 (adapted from (*Emissões setoriais de CO2eq., em Portugal, em 2022 | Relatório do Estado do Ambiente*, no date))

Portugal, by trying to stay on par with the EU trajectory, has facilitated the access to self-production systems, whether it is through economic incentives or by approving legislation that simplifies the process for everyone, from houses to industrial infrastructures. Laws for self-consumption and self-production are incapsulated in the *Decreto-Lei n.º 15/2022 | DR* (2022). In addition, and to facilitate the access to these information by the general population, the *Agência para a Energia* (ADENE) developed a legislative guide, that encompasses all the prevailing laws for self-consumption and renewable energy communities (REC) (ADENE, 2022). These laws are applicable to any self-producer whose electricity is destined for self-consumption, whether that occurs at the same location or not. It's also independent from connection to the public network. It must be based on RES. According to the National Plan for Climate and Energy, Portugal has the goal to consume 47% of its energy from RES (*Resolução do Conselho de Ministros n.º 53/2020 | DR*, 2020). Decentralized production, REC, and collective self-consumption is expected to play a big role in achieving this goal. The access to RES by the general public was made possible, in Portugal, by the decrease in in PV panels prices, as well as electrical storage and automation solutions. The main objective of the *Decreto-Lei n.º 15/2022 | DR* (2022) is to obey the EU directive that states that countries must facilitate self-consumption of energy and RES communities. Even non-domestic consumers can become self-consumers, as long as it doesn´t constitute their main professional activity.

According to ADENE (2022), there are different types of self-consumption: individual (ISC), which consists of a single delivery point, that can sell or not the excess energy to the grid; and collective (CSC), which is composed of multiple points of consumption, derived from a singular point of production and, similarly to ISC, excess energy can or not be sold to the grid. In a CSC, distribution can occur through an internal network or by using the public service electrical network. It's usually shared by infrastructures situated in close proximity. In fact, proximity between the producer and the consumers is a requirement. For connections through low-tension lines, the maximum distance is 2km or connection to the same transformation point; for medium-tension lines it is 4km; for high-tension lines is 10km; and for very-high-tension lines it's 20km. Each self-consumer is subjected to an extensive list of rights and duties that are forced to fulfil, as illustrated in Figure 6.

A renewable energy community (REC) is a collective person, whose members are located in close proximity to the RES projects, said projects belong to the REC or by third parties (as long as it is in benefit of the REC), and that the REC has, as its main objective, to give environmental, social, and economic value to the society, instead of financial profits. REC has the capability of producing, storing, consuming, buying, and selling renewable energy; share and sell the produced energy between the members; and access all of the energy markets.



Rights

- Install one or more self-consumption production units
- Establish and operate direct lines
- Establish, acquire, or operate a closed distribution network
- Consume the electricity produced or stored in their locations
- Buy and sell energy through energy markets or bilateral contracts
- Pay taxes and other faires
- Operate storage units

Duties

- Obtain a control title
- Support costs associated with the connection of the internal unit with the general grid
- Pay the designated prices when purchasing energy from the grid;
- Guarantee that the production unit has a size that is approximable to the needs of consumption, minimizing the excess energy
- Certify all equipments in use

Figure 6 - Rights and duties of a self-consumer in Portugal (adapted from (ADENE, 2022))

Inside a REC, share models exist between the units. The share models between the units are divided in different types of coefficients: fixed (only account for weekends and holidays, rarely account for seasons); variable (based on criteria defined by the ERSE); and mixed (as long as it is permitted by the legislation). Sharing may also occur via dynamic management, where monitorization occurs in real-time, with the intent of optimizing energy flows.

To install a unit, the person must communicate with the city hall the location of the equipment, the area of implementation, and a term of responsibility. Afterwards, depending on the installed power of the production unit, it may be required to acquire a license of operation, which also varies depending on the power. There are four categories for self-consumers: if it's less than 700 W, network injection is not allowed and there is no previous control required; if it's less than 30 kW, there needs to be a previous communication to the Collective Self-consumption Managing Entity (EGAC); if it's less than 1 MW, it is required to have a registration and an exploration certificate; and finally, if it's greater than 1 MW, a licence of production and exploration is mandatory. In addition to this, if the procedures require an environmental impact evaluation, then it's also needed to attain a licence for production and exploration. If there's a change of the installed power, that represents a change in category, then it is required a reemission of licence. Every eight years there's an inspection to verify the state of the equipment. For a unit with greater than 4 kW of installed power, it is obligatory to install 2 points of measurement: one of consumption/production (between the utilization unit and the grid) and a total counter (next to the production unit).

A self-producer must support all the costs associated with acquisition, installation, taxes, and exploration. They must pay to have access to all the required and appropriate networks at the voltage level. Although the utilization of internal networks is not subjected to any charge, the acquisition and installation of the network entails costs that have to be considered. However, the most recurrent share of costs will be with the electricity bought to the general grid. Unless the unit is fully self-sufficient, which is still rare, it will be required to purchase energy when the RES are not capable of meeting the demand. Portugal currently utilises the time of use (TOU) program, as seen in section 2.3. This is one of the most common approaches worldwide and is used in several papers (Wang *et al.*, 2019; Vahid-Ghavidel *et al.*, 2020). The price scheme may vary throughout the day, depending on the contractualised conditions. One of the most common is the four-hourly rate, as seen in Figure 7.

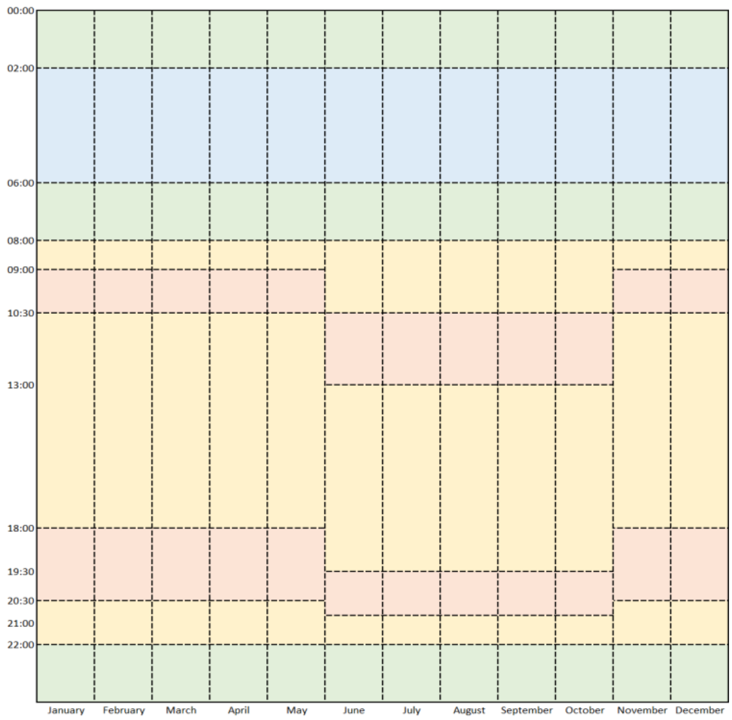


Figure 7 - Annual electricity tariffs in Portugal, daily cycle (*Tarifas e preços - eletricidade - ERSE*, 2024)

According to *Regulamento Tarifário - ERSE* (2023), this rate divides the year into two blocks, summer and winter, followed by a division throughout the day. In Figure 7, the green blocks represent the off-peak hours, where the energy price will be the lowest; the yellow blocks represent the mid-peak hours, an intermediate price range; the red blocks represent the peak hours, when the energy price will be the highest; and the blue blocks represent the super off-peak hours, only applicable to consumers who are connected to special low voltage, medium voltage, high voltage, or very high voltage, and when the price will drop to below off-peak hours.

The energy market can vary throughout the day, especially in real-time purchasing and selling. To adjust to this, some modelling tools already have built-in economic representation, some with elasticity, that can respond to fluctuations in the electricity price (Després *et al.*, 2015). As such, it is important to explore all the possibilities. Whether to sell, buy, store, or even exchange energy in REC, it is important to consider all of the viable options when making decisions.

3 Technologies and innovations

3.1 Solar Energy

According to data from the “Statistical Review of World Energy”, by the Energy Institute (2024), the world produced more than 1,600 TWh through solar energy in 2023. As seen in Figure 8, since 2010, solar energy has had an exponential rise, becoming the third biggest RES producer of energy. However, it still presents a lower intensity than hydro and wind, and production is not homogeneous throughout the globe, as evidenced by the map present in Figure 9.

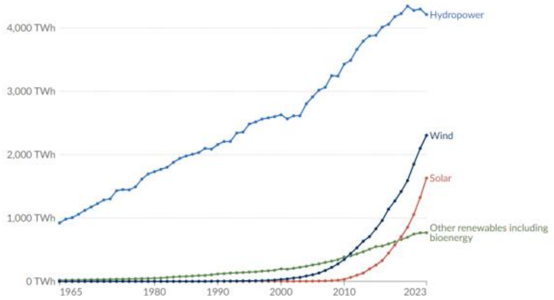


Figure 8 - Renewable energy generation by source (adapted from (*Solar power generation*, 2024))

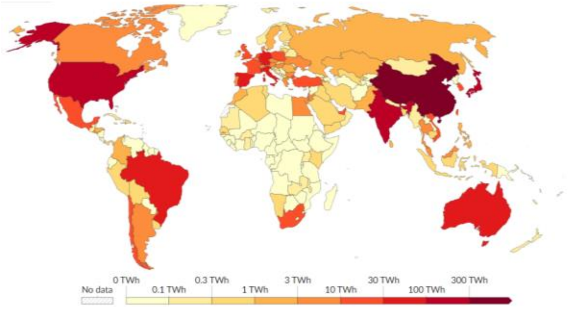


Figure 9 - Solar power generation in 2023 (adapted from (*Solar power generation*, 2024))

An estimation of the average energy production through solar energy can be estimated via global irradiance (Colacicco and Zacchei, 2020). According to Cao and Lin (2008) solar irradiation has two main parts: a fixed part, consisting of the effects caused by seasons, dates, time, and geographic location; and random part, which is the most difficult to predict, consisting of the effects caused by the weather and the surrounding conditions. An example of this type of random prediction objects is cloud cover, that is not only hard to predict but also hard to describe in a numerical scale with great precision. Long enough time periods will show that solar irradiance is repeatable. However, shorter time series will show that the data is highly stochastic (Alzahrani *et al.*, 2017). The meteorological variability experienced by one area can be offsetted by the conditions in another area (Fisher *et al.*, 2013, cited in Devlin *et al.*, 2017).

According to Pandey *et al.* (2021), solar power can be used for different treatments of wastewater. It has a gross potential of 600 terawatt with technical feasibility of 10% of the entire gross potential. However, the current installed capacity of solar power is only 0.005 TW. Developments are continuous in this area: parabolic through systems, central tower systems, dish solar systems, Fresnel reflectors, solar photocatalysis, water heating, solar desalination, solar distillation and disinfection, solar detoxification, solar pasteurisation, and ultraviolet radiations (used in solar detoxification process for breaking down contaminant molecules) are some examples of technologies that utilize the Sun as a source of energy and have seen development in the last twenty years (Foley, 2010; Bustamante and Liao, 2017; Pandey *et al.*, 2021).

Another technology that uses solar energy as a RES is solar still. As defined by Zarasvand Asadi *et al.* (2013), it is a "green energy process that uses the free natural energy of the sun to purify contaminated water to produce clean water. Uses the solar energy instead of other sources of energy like fossil fuels, oil, and gas to gain the energy needed for purification”. The main advantages of using the solar still process are that a solar still has no moving parts and the used energy is renewable, free, and clean. Alvarez-Guerra, Dominguez-Ramos and Irabien (2011) focused on electrochemical oxidation based on boron-dropped diamond (BDD) and photovoltaic solar electro-oxidation (PSEO). BDD represents a high investment and has a high operational cost. PSEO consists of the direct integration of PV in the electrochemical reactions. Shows a reduction of economic and environmental impacts and has increased autonomy. It is an attractive technology for wastewater treatment and does not require batteries. The study concluded that a PSEO installation's feasibility is directly intertwined with the geographical location of the installation, with lower irradiation meaning lower productivity. Fernandes *et al.* (2009) provides an in-depth approach to solar thermal and solar thermoelectrical technologies. The first one consists of a solar collector that converts solar energy into thermal energy, through the heating of water, air, or other thermal fluid. Its use is extremely scattered, with some countries such as Germany, Austria, or China, investing heavily in this technology, whilst being rarely used in other countries. Most commonly it’s used as a decentralized form of production. Solar thermoelectric energy is produced in solar power towers, using solar radiation concentrators. It is mainly used in centralized production. Spain, North Africa, North America, and Australia are some of the leaders in developing and utilizing this technology.

The most used technology to produce electricity from solar energy is PV. PV's main advantages reside in using one of the most widespread RES, has high energy productivity potential, presents environmental benefits (low fossil-fuel consumption and low CO_2 emission), is based on self-consumption, since the input energy form is free, and is widely available to anyone (Colacicco and Zacchei, 2020). Odabaş Baş and Aydınalp Köksal (2022) performed an analysis of WWTPs with high energy consumption in Türkiye. For PV, results showed that, even without selling energy to the general grid, it can still be integrated into WWTPs with a flow rate of 10 to 50 million cubic meters per year. The only scenario in which it wasn't cost-effective was for small scale WWTPs. However, Strazzabosco, Kenway and Lant (2019) found no significant correlation between the flow rate of the WWTP and the capacity of the PV system installed in the study of 569 plants in California. Furthermore, the study stated that lack of biogas recovery opportunity and land availability were the two main reasons to adopt a PV system in a small scale WWTP. Colacicco and Zacchei (2020) studied a WWTP in the Mediterranean area. It was presented a correlation between the fluctuation of air temperature throughout the year, which affects the temperature of the wastewater, and the production of electricity through PV. It's proved in the paper that PV is a good solution for the high energy consumption problem in WWTP. Rosa-Clot, Tina and Nizetic (2017) analysed the impact of a floating PV system on the evaporation rate of water, due to the increased shading and reduced wind effect. The installation presented competitive costs when compared to a land-based PV installation, with the payback time situated in the range of 3 to 4 years. Overall, it can lead to cost reduction and an improvement of the environment, due to the smaller amount of evaporated water. Although PV is often utilized to convert radiation from the Sun into electricity, as an intermittent power source (Foley, 2010), it can be coupled with other technologies. An example of it was the case presented by Mendecka *et al.* (2021), which coupled PV with an unitized regenerative solid oxide fuel cell (URSOFC). It functioned as a fuel cell and an electrolyser with relative success. Chae and Kang (2013) studied the feasibility of using RES in a WWTP in Korea. In addition to a small hydropower station, a PV system with a total capacity of 100 kW was analysed. Simulation results show that a 96 kW PV installation was estimated to produce 150.7 MWh/year. 100 kW produced a maximum of 155 MWh/year. Coated panels produced 6% to 8% more power, making it important to keep the panels clean. Overall, the total production ascended to 7554 MWh/year, with 98% being electrical. Energy independence was of 6.5%, with less 261ton CO_2/year emitted.

3.2 Biogas

Throughout literature, multiple definitions for biogas can be found. According to Fernandes *et al.* (2009), biogas results from the process of anaerobic digestion. Due to the action of bacteria, organic matter decomposes, turning into a gaseous mixture that can be stored until necessary. This mixture, according to Masłoń *et al.* (2020) is mainly composed by methane and carbon dioxide, with trace amounts of hydrogen and nitrogen. To produce biogas, waste, such as sewage sludge, is used, transforming it into this alternative source of energy (Silvestre, Fernández and Bonmatí, 2015; De Vrieze *et al.*, 2016, cited in Masłoń *et al.*, 2020).

Integrating biogas in a WWTP can be easily done due to their high potential and rich organic content of wastewater, ease of storage, and high production stability (Masłoń *et al.*, 2020; Odabaş Baş and Aydınalp Köksal, 2022). As seen in Figure 10, biogas requires a gasifier or digester to be produced (Kasaeian *et al.*, 2019). After being produced, biogas is stored. Instead of storing electricity, which can be costly especially at a high level of energy demand, the WWTP can instead store gas (Fan *et al.*, 2021). When required, biogas can be retrieved from the storage to produce energy. The amount of energy generated from biogas is dependent of the size of the plant, the treatment level, and the technology adopted to generate electricity from biogas (Strazzabosco, Kenway and Lant, 2019). Biogas production can be increased through the implementation of an anaerobic co-digestion process, improving stability and efficiency in the anaerobic digestion process (Masłoń *et al.*, 2020). When the storage is completely full and there is no opportunity for production of energy, the WWTP has no option other than burning the excess gas in the torch.

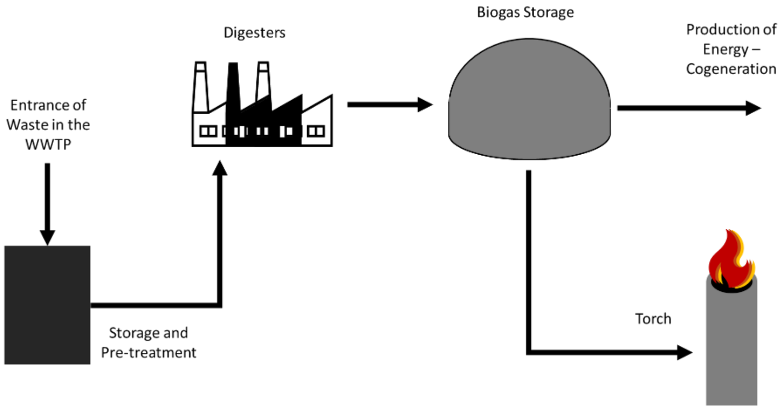


Figure 10 - Biogas production scheme in a WWTP

To be transformed into energy, a WWTP utilizes cogeneration/trigeneration technologies (Li *et al.*, 2021). While there are some production units that utilize combined heat, cold, and power (CCHP), the most common approach is the use of combined heat and power (CHP) (Møller Sneum, 2021). A CHP can supply heat and electricity from the same source of energy, in simultaneous (Cao *et al.*, 2018; Bagherian and Mehranzamir, 2020; Fan *et al.*, 2021). It was commonly used to fulfil electricity and heating demands, having been transformed into a flexibility provider while satisfying heating and electricity demands (Bagherian and Mehranzamir, 2020). As stated by Devlin *et al.* (2017), gas fired power stations are much better at adapting to the irregular production than other RES. CHP has a higher fuel economy and efficiency than separate systems (Cao *et al.*, 2018). It is characterized by having low emissions, especially when compared to coal and oil (Devlin *et al.*, 2017). Piacentino *et al.* (2013) and Bagherian and Mehranzamir (2020) reinforced the importance of CHP in the reduction of GHG emissions, increase of efficiency, lower fuel consumption, and overall energy savings.

Even though biogas has been used since 10th century B.C. (Bond and Templeton, 2011), new studies and technological advances are still made, especially for their applications in WWTPs. Odabaş Baş and Aydınalp Köksal (2022) analysed the impact of market-based instruments in WWTPs in Türkiye. Results showed that biogas integration is not cost-effective without a CO2 penalty, although, with increased incentives, the payback period decreases. Even with three times the necessary energy production, only 88% of it was for self-consumption, due to storage and CHP limitations. Bustamante and Liao (2017) faced a negative energy balance when utilizing biogas, due to the high energy demands of the aerobic treatment required, which could not be offsetted by the energy produced from anaerobic digestion. According to Strazzabosco, Kenway and Lant (2019), five million gallons per day of flowrate is the threshold size to guarantee economic feasibility of using biogas for CHP in a WWTP in California, since biogas increases production with the increase in size of the WWTP. Helal, Ghoneim and Halaby (2013) used activated sludge treatment process and achieved a 69% coverage of the WWTPs peak load. Li *et al.* (2021) encountered difficulties interconnecting biogas with electricity, when modelling an IES, due to the fact that gas is transported at a much slower rate than electricity and has a higher inertia. Similarly, when modelling an IES, Cao *et al.* (2018) met resistance from CHP, due to the fact that it produces heat and electricity at the same time, it requires different sets of constraints to be applied simultaneously, such as outages of lines and generators, uncertain demand and generation, and uncertainty of fuel prices and environmental policies. Bongards *et al.* (2014) utilized ML to optimize a substrate mix for biogas production. It was tested over 19 weeks and resulted in improved biogas and power production.

The application of biogas must be studied for every case, since different conditions can lead to different necessities to reach economic feasibility. However, it is impossible to understate the importance of biogas for GHG emissions reduction. According to Fernandes *et al.* (2009) many countries already have invested in this technology, especially in Europe, which has led to it gaining importance and value worldwide.

4 Methodologies

4.1 Case study

The case study analysed consists of a WWTP in *Vila Nova de Gaia*. The simplified scheme for the WWTP is presented in Figure 11. The WWTP has production of biogas, which is used for the production of electricity and heat in a CHP. Additionally, it has the capability of storing biogas in a gasometer, with a maximum capacity of 1250 m^3. Complimentary, a PV installation is also being added to the system. It is composed by 888 modules and has an estimated maximum capacity of 488 kWp. A total of five inverters will also be installed in the system and the overall estimated performance ratio is estimated to be 88.21%.

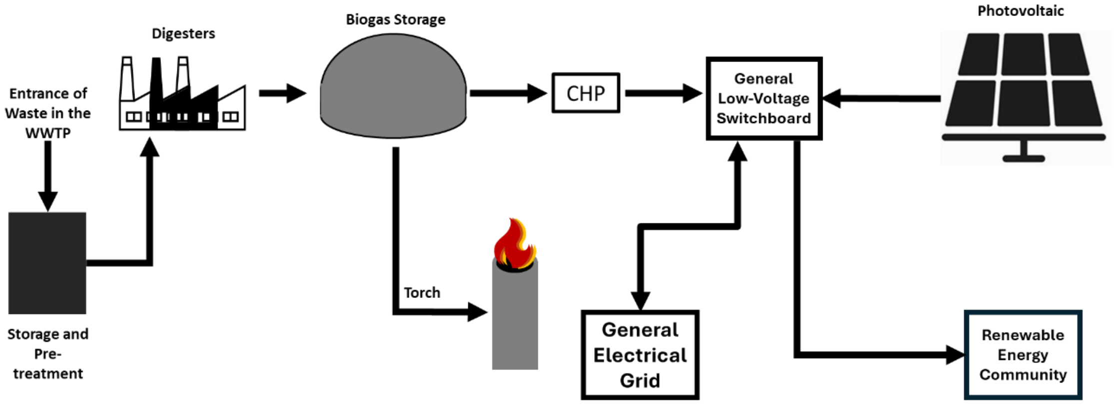


Figure 11 - Functioning scheme of the *Gaia Litoral* WWTP

The WWTP is connected to the general electrical grid, allowing for the possibility of not only buying energy from the grid, but also sell it or even create a REC. As stated in section 2.4.1, a REC can be established with other parties integrated in the same collective person, depending on the voltage and the geographical distance. The map present in Figure 12 shows the infrastructures that belong to SimDouro. Additionally, the three circles show the infrastructures that are situated at less than 2, 4, and 10 kilometres of the *Gaia Litoral* WWTP. As shown, there are three pumping stations in less than a two-kilometre radius, five pumping stations inside the four-kilometre mark, and inside the ten-kilometre mark there are sixteen pumping stations and two WWTP.

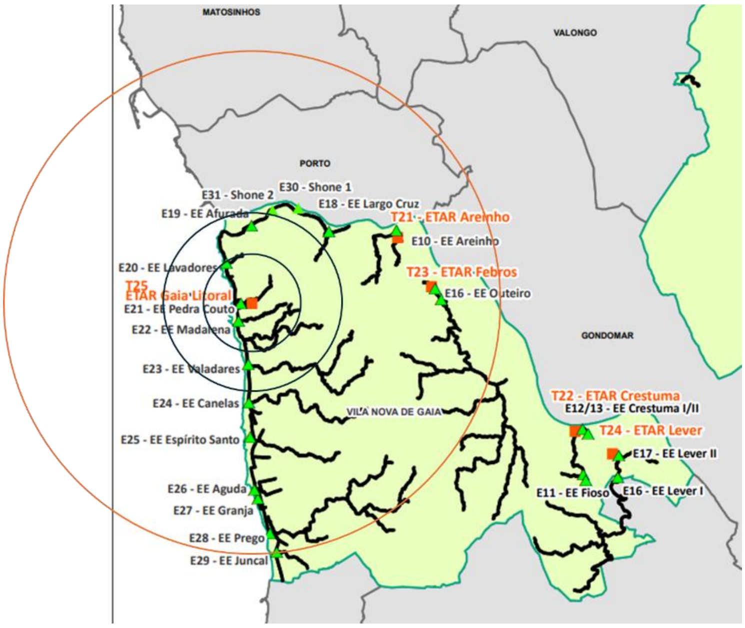


Figure 12 - Map of the infrastructures belonging to SimDouro. With triangles are marked the locations of the pumping stations and with squares are marked the WWTP.

4.1.1 Objectives

This study will have two main aspects to it: the first one will consist of optimizing the utilization of the available sources of energy by the WWTP; the second one will entail of an economic analysis of the investment possibilities in the plant. For both cases, solutions will be presented and scrutinized with the appropriate tools.

In the case of the optimization problem, three main objectives are proposed: minimize the burning of biogas through the torch; reduce the costs associated with buying energy from the grid; and finally, achieve, if possible, self-sufficiency. For the first two objectives, which are priorities, will be attended via individual simulations, with the purpose of achieving the best possible result on each variable. Afterwards, a compromised model will attempt to achieve the best solution for the two variables simultaneously. The third point, referring to self-sustainability, will be analysed as a byproduct of the other points, not requiring a specific simulation or model for it. The minimization of the burn of biogas is essentially related to an environmental aspect. While burning, the process destroys fuel and releases GHG to the atmosphere. The remaining points are mostly related to an economic standpoint, with the focus residing on avoiding unnecessary costs for the WWTP.

For the economic analysis, the main objective is to assess the potential for an investment in a second CHP unit, in order to utilize the excess biogas and subsequently eliminate the need for burning fuel. Additionally, an analysis of PV viability for the WWTP is also carried out. This study was deemed important due to the fact that the biogas production in the plant is usually higher than the energy needs, as shown in the graphic of Figure 13. This becomes particularly relevant due to the decision taken by the WWTP of not implementing any storage for the energy produced by the PV.

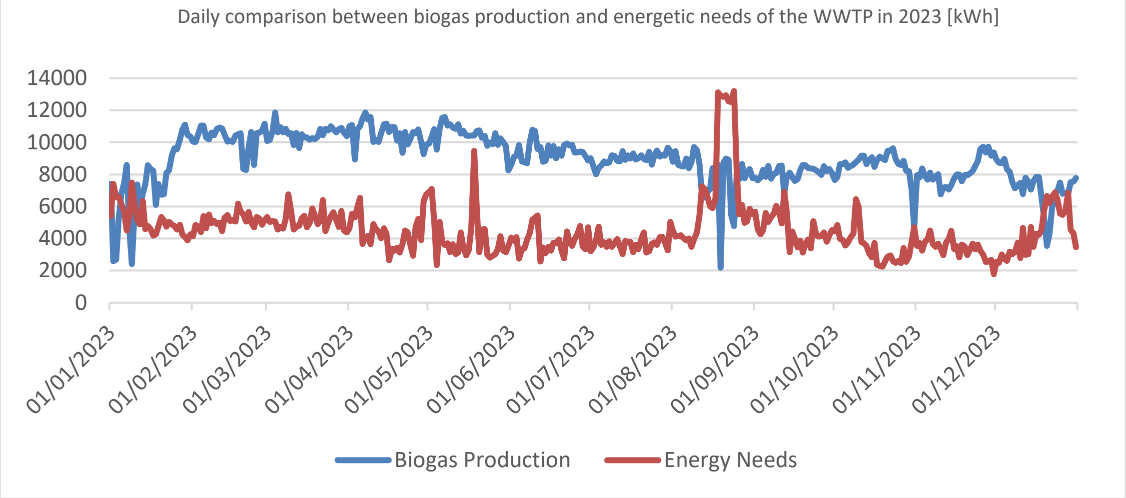


Figure 13 - Daily comparison between biogas production and energetic needs of the WWTP in 2023 [kWh]

4.1.2 Constraints and assumptions

In a system as complex as this WWTP, it is bound to exist constraints in multiple areas. As mentioned in section 4.1.1, batteries or other forms of storage for the energy originating from the PV setup were not considered. This was due to a prior imposition of the company, related with economic and spatial limitations and previous studies developed.

Naturally, the existing equipment also has boundaries. The gasometer volumetric capacity cannot exceed, at any given moment, the 1250 m^3. After this volume is hit, the additional biogas is obliged to either be directed to the CHP to be converted to heat and electricity or be redirected to the torch to be burned. The CHP has an existing maximum capacity of roughly 500 kWh, while the PV system has a maximum capacity of 488 kWp. Although the WWTP has capacity to install more PV modules, the company is limited to a 1 MW total electricity production capacity, before ascending to the next step in the Portuguese legislation, as explained in section 2.4.1. The PV system is also not subject to any changes and should maintain the pre-determined characteristics.

Some assumptions were also made throughout the work. In the CHP, only the electricity output will be considered. Although the biogas that enters the CHP will also produce heat, this is disregarded. For the biogas data analysis, it will be considered that the volume inside the gasometer started at zero on the first day of the year. In this case the volume inside the gasometer has to be build up in the early stages of optimization. Finally, for the economic assessments, when calculating the cash-flows, it will be considered a constant annual cash-flow throughout all the year of investment.

4.2 Modelling approach

After analysing the approaches used in literature, as stated in section 2.2.2, and the necessities of the WWTP, the selection fell on a rule-based approach implemented in Microsoft Excel, as used by Mendecka *et al.* (2021). This decision was due to the fact that, as mentioned in section 4.1.1 and seen in the graphic of Figure 13, biogas production is consistently enough to satisfy the energetic needs of the WWTP. This leads to a frequent scenario in which the PV system will be used to feed electricity in a REC or to generate profit via selling energy. The only scenarios in which PV use for the WWTP is justified is when biogas production diminishes, due to a malfunction of an equipment for example. It is not expected that the production of biogas suffers massive fluctuations in regular conditions, since it derives from incoming waste. PV can also be used to replenish the volume of biogas inside the gasometer when the reserves are low. This leads to a straightforward modelling approach, in which PV produced electricity is often redirected towards the outside of the WWTP. This method also brings the additional advantage of requiring low computational resources and is able to produce results in a shorter time frame, making it viable for short-term optimization. To first design the flowchart for the problem, Microsoft Visio is used. This is a tool dedicated to diagramming and vector graphics, capable of creating accurate projects.

In opposition to the traditional approach when optimizing an IES, the main energy source for this project will not be the PV, but instead the biogas. This decision is justified, firstly, by the defined objective of reducing the biogas burned in the torch; secondly, by the lack of storage on the PV side, in opposition to the gasometer, that requires closer management throughout the day; lastly, by the previously mentioned fact that the biogas production is not only stable but also consistently superior to the energetic needs of the WWTP.

4.2.1 Model limitations

Although the model choice presents clear advantages when compared to others, it still has some drawbacks. The rule-based approach, in this scenario, will be better suited for smaller time-steps optimization. However, and even though it is functional, real-time optimization should be avoided with this type of model, since it can result in fast switching between rules when close to a border of decision. Longer time-steps will have the opposite effect, resulting in errors and malfunctions due to the high spacing between possible rule changes, becoming less adaptable and more susceptible to generate solutions further away from the optimum one. Short time-steps will be favourable, enabling the ability to backtrack and alternate between conditions without missing important information and variations in production. As such, the recommended time-step is between fifteen minutes and one hour. In this work, the time-step used will be of one hour, to accommodate the existing data in the best way possible.

The rule-based approach, in spite of its simplicity when compared to ML, requires an extensive amount of work in the initial stages. The design of the command flowchart is an important step to ensure the flexibility and efficiency of the model. By nature, it will lack in adaptability when compared to the remaining models, requiring restructuring when there is a drastic change in the conditions and environment surrounding the plant. Whilst ML requires a large dataset to operate, this is not the case with the rule-based approach. However, to establish solid conditions and boundaries, it is important to have a deep understanding of the system responses, energy availability, and energy needs of the WWTP, thus making the existence of a solid dataset crucial.

4.3 Photovoltaic forecast

To accurately estimate the overall production of energy from the WWTP, it is fundamental to forecast PV production. This is an arduous task that requires advanced programming and extensive datasets. Instead of it, an alternative was found to suppress the needs of the model, the Solcast API Toolkit. It contains predictions for the following 14 days, with timesteps ranging from 5 to 60 minutes (*Solar Live & Forecast Data API | Solcast^{TM}*, no date). The forecasts include cloud opacity, solar geometry, albedo, PV power, global horizontal irradiance (GHI), among other variables, making it a versatile and useful tool for PV output prediction. Additionally, it also provides a database that tracks back until 2007. In this, historical time series can be requested with radiation and weather data, with the same timesteps available. This is particularly important when testing with data from previous years. In this case, when utilizing biogas and consumption data from 2023, extra data from Solcast will be used to estimate solar PV production during the respective time period, given that the installation of PV panels was still non-existent. The extracted data will also have an hourly timestep, in order to best match the existing data. This will allow for a fair comparison of the results obtained and testing of the models developed.

As stated in section 4.2, Microsoft Excel will be used as the basis for model. As such, Power Query is used to integrate data, whether it is from an already existing Excel file, or to extract data from online databases in real-time. Before settling for the aforementioned solution, tests were made with other databases such as Weather Underground or Weather Channel. Data from these sources, although not used in the final models, were not discarded, and are used as a comparative factor to ensure the quality of the data derived from the Solcast engine.

The location of the WWTP is a critical piece for estimating PV production. As such, geographical data needs to be retrieved in order to correctly calculate the final output. For that purpose, the approximate coordinates of the plant are retrieved using Google Maps, as shown in Figure 14. According to it, the latitude is 41.11183 and the longitude is -8.65491. According to a previous study developed by the company, the azimuth is considered 0°, the tilt angle is set at 30°, and the performance ratio or efficiency factor is estimated to be 88.21%.

For forecasting purposes, Solcast is capable of directly predicting the PV output, if the system is smaller than 1 MW peak output. It requires the coordinates, capacity of the system, azimuth, tilt angle of the panels, and the efficiency factor of the PV system. For previous data, calculations were required to achieve the value of PV production per hour. For each day of the year of 2023, it is necessary to calculate the solar declination angle (δ_S). The equation 1 is used, which was first introduced in Cooper (1969) (cited from El Mghouchi *et al.*, 2016):

$$\delta_S = 23.45 * \sin\left(360 * \frac{284 + N}{365}\right) \tag{1}$$

, where N is the day of the year.

Figure 14 - Coordinates of the WWTP of *Gaia Litoral* (adapted from *Google Maps* (2024))

Afterwards, it is necessary to calculate the true solar time (TST). However, to calculate the TST, it is mandatory to calculate the B variable, described in equation 2, and the equation of time (in minutes) ET, shown in equation 3, as described by Yousef *et al.* (2023). Lastly, TST (in minutes) is present in equation 4:

$$B = (N - 81) * \left(\frac{360}{364}\right) \tag{2}$$

$$ET = 9.87 * \sin(2B) - 7.35 * \cos(B) - 1.5 * \sin(B) \tag{3}$$

$$TST = LT + ET \pm 4 * (|\lambda_{timezone}| - |\lambda_{local}|) - DS \tag{4}$$

, where N is the day of the year; LT is the legal time, $\lambda_{timezone}$ is the longitude of the time zone by which the area is structured, which, in the case of Portugal, that is governed by the

Greenwich Meridian, is 0; λ_{local} is the longitude of the location, as determined above, is negative 8.65491; and DS is daylight savings, which should only be applied when daylight savings are being used, and consists of the subtraction of 60 minutes to the TST.

In order to calculate the hour angle (H), which is the following step, equation 5, extracted from El Mghouchi *et al.* (2016) and Alam Emon, Ahmad and Hasanuzzaman (2022), was used:

$$H = 15 * (TST_{hours} - 12) \tag{5}$$

, where TST is the previously calculated true solar time, converted to hours.

The next step is the calculation of the zenith angle (h), which follows the formula patented in Kaddoura, Ramli and Al-Turki (2016) and shown in equation 6:

$$\sin(h) = \sin(\delta_S) * \sin(\phi) + \cos(\delta_S) * \cos(\phi) * \cos{(H)} \tag{6}$$

, where δ_S is the solar declination angle; ϕ is the latitude of the geographical location; and H is the hour angle.

Afterwards, it is necessary to calculate the plane of array irradiation (PAI), which can be done by applying equation 7:

$$PAI = GHI * \cos(h) * \cos{(\alpha)} \tag{7}$$

, where GHI is the global horizontal irradiance; h is the zenith angle; and α is the panels tilt angle.

Finally, in equation 8, it is possible to estimate PV production:

$$PV_{production} = PAI * \mathrm{A_p} * PR * \eta \tag{8}$$

, where PAI is the plane of array irradiation; $\mathrm{A_p}$ is the total area of installed PV panels; PR is the performance ratio; and η is the efficiency of the system, which was arbitrated to be 20%.

By following this sequence of equations, it is possible to obtain an estimate of the hourly PV production during the year of 2023, of an installation with similar characteristics to the ones of the system currently in installation and assess the impact not only on the optimization but also on the economic front.

4.4 Optimization

To execute the required simulations, and as stated in section 4.2, it is used the Microsoft Excel software. In combination with it, Visual Basic for Applications (VBA) and Power Query, tools that are incorporated in the Excel environment, are also required. The first one is a simple yet powerful programming language, that is used, in this scenario, to write the required code and run the desired simulations. The latter is a tool designed for data extraction and transformation.

It is useful to compile multiple sources of data into queries, before importing them directly into Excel. While some calculations are easily made in Excel, the bulk of the modelling has to be executed in VBA. This is due to the necessity of implementing *if statements* and *do while functions* in chain, to replicate the order derived from the flowchart.

For the initial approach, variables have to be defined. These will represent the movements of energy throughout the WWTP in varied forms: electrical energy, volume, and flowrate. In Figure 15, variables are added to the WWTP's functioning scheme, which are explained in the following bullet points:

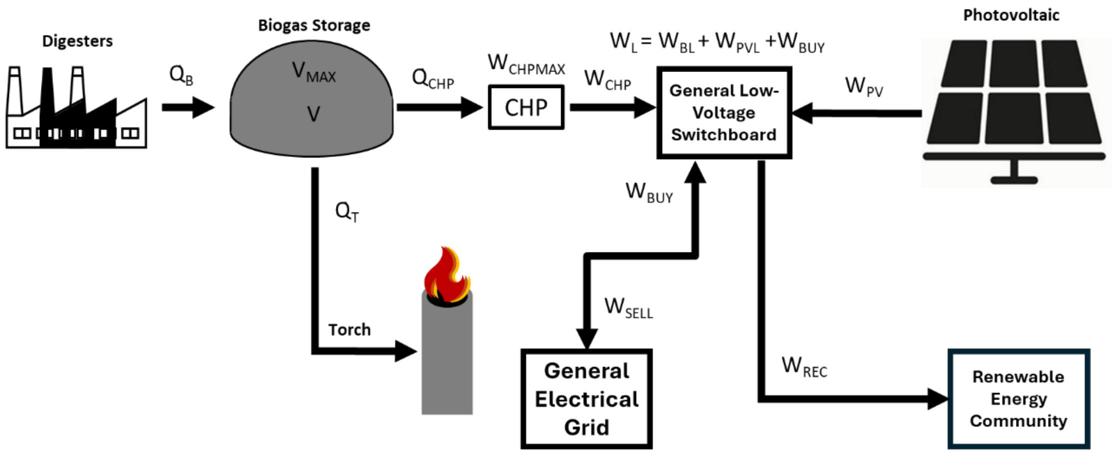


Figure 15 - WWTP functioning scheme with variables

- $\dot{Q}_B$: flowrate of biogas being produced at any given time; it is forced to be sent to the biogas storage.

- V: volume of biogas present in the gasometer at any given moment; it has a subsequent variable, V_{MAX}, which represents the maximum capacity of the gasometer (1250 m^3); the biogas inside the storage can either be kept inside it to be used in a more opportune time, be forwarded to the CHP, or be expelled through the torch.

- $\dot{Q}_T$: flowrate of biogas forwarded to the torch; comes from the biogas storage, when the storage has been exhausted and no extra biogas can be stored; it is one of the main variables to be minimized during the optimization problem.

- $\dot{Q}_{CHP}$: flowrate of biogas sent towards the CHP to be converted to electricity and heat.

- W_{CHP}: electrical energy produced by the CHP; it has an indexed variable, W_{CHPMAX}, which represents the maximum electrical energy that the single CHP can produce at a given time; the produced electricity has to be used by the WWTP, sold to the general electrical grid, or sent towards the REC.

- W_L: electrical energy load of the WWTP; consists of the energetic needs of the plant at a given moment; it must be always satisfied; can be decomposed in the sum of the electrical energy from the biogas side (W_{BL}) with the electrical energy from the PV side (W_{PVL}) and the bought energy from the grid (W_{BUY}).

- W_{PV}: electrical energy produced by the photovoltaic installation; it is heavily dependent on the weather conditions and irradiation values; once produced, electricity must either be used by the WWTP, donated to the REC, or sold to the general grid.

- W_{BUY}: electrical energy bought by the WWTP from the general grid to suppress their needs when the sum of W_{PV} and W_B are insufficient; it is directly connected to another variable, $€_{BUY}$, which is the cost at which the energy is bought; this cost is variable throughout the day and the year, requiring a careful and planned approach to ensure cost minimisation; it is one of the variables to be minimised during the optimisation process.

- W_{SELL}: electrical energy sold by the WWTP to the general grid; it is one of the possible channels for excess energy to be disposed of; it is directly connected to another variable, $€_{SELL}$, which is the cost at which the energy is sold to the grid; the price must be contractualised between the WWTP and the energy provider and it may vary throughout the day and year; currently, since no contract exists, the price is set at 0 €/kWh, which in essence translates to the energy being donated to the grid with no monetary benefit for the company.

- W_{REC}: electrical energy given by the WWTP to the REC; it is the other option to dispose of excess energy in the plant.

To test the developed models, data from 2023 will be used, in conjunction with the PV estimations calculated as described in section 4.3. The data is pre-processed according to the research presented in section 2.2.3. As stated in the start of the present section, the objectives are already defined, as is advised throughout the presented literature. The time-step must be equal throughout the entire dataset. As such, a one-hour time period was selected, and data is appropriately adjusted. Biogas data from 2023 had a one-day time period, requiring an assumption, dividing the biogas value equally throughout the day. This may not reflect precisely the existing conditions, but, since biogas production is recurrent throughout the entire day, it is considered a solid approximation. On the other hand, PV data extracted from Solcast has a 30-minute time period. In this case, the solution is much simpler and accurate, given that, for each hour, two 30-minute time periods can be directly summed to obtain the hourly estimation for PV production.

As shown in Figure 7, the purchase prices of electricity are directly linked to the hour of the day and the month of the year. It is categorised into two periods and four categories, for the four-hourly tariff: peak, mid-peak, off-peak, and super off-peak. The prices corresponding to each category and period, as well as the respective percentual increase in price between categories is shown in Table 1. This information is crucial to guarantee the best possible optimization outcomes. It has to be linked to the respective hour, in order to automatically determine the price for any given hour. In the cases in which the price changed during the hour, the considered price is the highest of the two.

Table 1 - Categorization of energy purchase prices (adapted from *Tariffs and prices - electricity - ERSE*, (2024))

Period	Category	Energy purchase prices	Price increase by category
Winter (November through May)	Peak	0.1205	6%
	Mid-Peak	0.1138	14%
	Off-Peak	0.0984	10%
	Super Off-Peak	0.0882	
Summer (June through October)	Peak	0.1109	2%
	Mid-Peak	0.1084	12%
	Off-Peak	0.0959	3%
	Super Off-Peak	0.0932	

Afterwards, the existing data is transposed to the main simulation Excel spreadsheet. Simulations are run in the VBA environment, where the code to execute them is written. The code will automatically fill the spreadsheet with the results obtained. Since there are different forms of energy translated in the system, with biogas being expressed in m^3 or m^3/h (volume or flowrate), while the remaining electrical energy is expressed in kWh. To account for the necessity of comparing these two different units, a conversion factor is adopted. According to Groeneveld (2022), on average, a cubic meter of biogas can produce 2 kWh of electricity. According to the WWTP, the estimate made is for 6 kWh/m^3 with 38% of efficiency, which results in an overall conversion factor of 2.28 kWh per cubic meter of biogas. To further verify this conversion factor, data was retrieved from the WWTP referring to the year of 2023. In this year, the total electricity produced by the CHP was of 2,798,700 kWh. For the same period, 1,192,131 m^3 of biogas entered the CHP. By dividing the two values, a 2.348 conversion factor is achieved. With all of this information, the values given by the WWTP are given priority, and the conversion factor adopted is 2.3 kWh per cubic meter of biogas. Thus, for every necessary conversion between volume and electricity, this will be the used conversion factor. Three optimization scenarios were projected: the first one focuses on keeping the burnt biogas to a minimum; the second one focuses on avoiding the purchase of energy of the general grid; and the final one is a compromise between the two previous models, designed to obtain a middle of the road solution.

There are four main metrics of analysis for the results obtained in the simulation portion of the work. The first one is the amount of biogas burned in the torch ($\dot{Q}_T$). This value should be reduced when compared to the values without the optimization mechanisms. The second one is the amount of energy purchased and the total cost of purchased energy. Similarly to the previous one, this should also strive to be the minimum possible value and should present a reduction in comparison with the results pre-optimization. The self-sufficiency ratio (SSR) will also be calculated to compare with the results pre-optimization, as presented in equation 9. Contrary to the previous two, the SSR should be the closest possible to 100%, which would translate into full self-sufficiency of the WWTP. Lastly, the ratio of wasted biogas, which will quantify the burnt biogas in comparison to the produced biogas per year is shown in equation 10.

$$SSR = \frac{\sum Consumed - \sum Bought}{\sum Consumed} \tag{9}$$

$$Wasted\ Biogas = \frac{Q_{torch}}{Q_{biogas}} \tag{10}$$

4.5 Economic analysis

In the economic analysis, and as stated in section 4.1.1, the main objectives are to analyse the economic viability of installing a second CHP unit in the WWTP and the economic impact of the implementation of the PV system. The second CHP unit, as shown in Figure 16, would be implemented in parallel with the first CHP unit, and its main purpose is to increase the capacity of production of electricity through biogas. This will lead to a reduction in the usage of the torch and, consequently, reduce the amount of burned biogas.

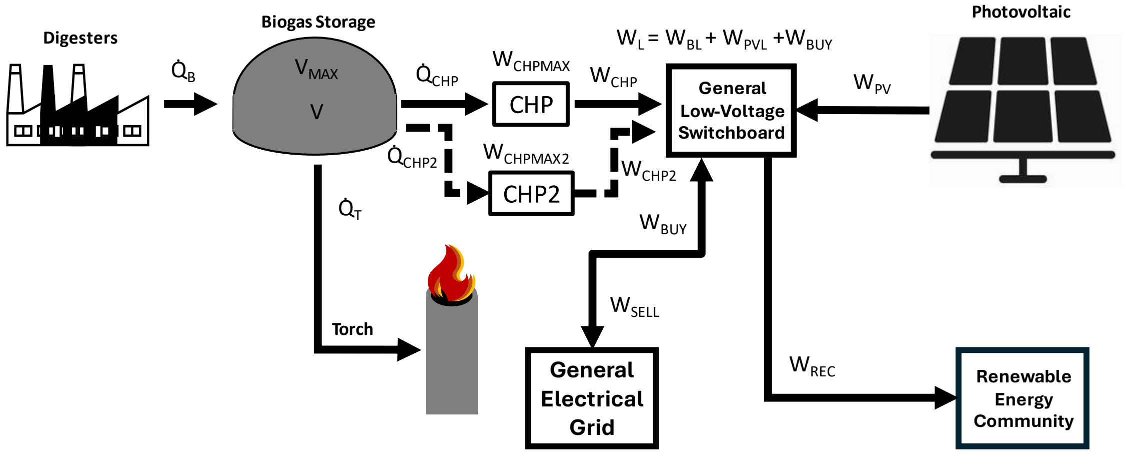


Figure 16 - Functioning scheme of the WWTP with a second CHP unit

The first step is to determine the maximum power that the new CHP should have. This will be based on the value of burnt biogas in the torch, $\dot{Q}_T$, and it will be used the conversion factor between cubic meters of biogas and electricity, stated on section 4.4. The power of the CHP will vary according to the results obtained in the simulation. This step will be followed for three scenarios: the first scenario will utilize the biogas data from 2023, with the assumption that the volume inside the gasometer starts at zero and then progresses through the year; the second scenario utilizes biogas and PV data and the optimization method is focused on avoiding buying energy; the last scenario is similar to the previous one, with the difference residing on the focus of the optimization approach, that is focused on minimizing the burnt energy through the year.

The next logical step is to estimate the costs of each component. According to *6.8 Cost of CHP: Engineering and Installation Costs* (no date), the average installation cost for a CHP is between 1123 €/kW and 3000 €/kW for a gas turbine, with a 69% average CHP efficiency. As for the cost of the electricity bought to the grid, the exact values are shown in Table 1.

In the second part of this economic analysis, the objective is to assess the advantages of implementing a REC or selling the excess energy to the grid. Currently, the WWTP is only able to donate energy to grid. In essence, the only current upside is to drain the excess energy and avoid safety hazards on the general low-voltage switchboard. However, the simulations are made to determine the lowest sell price that will allow for a capital recovery period (CRP) smaller than 10 years. For the REC implementation, the energy donated via this method will be used by other infrastructure of the same company, instead of it purchasing electricity from the grid. So, even though the energy will leave the WWTP for free, it will result in savings equivalent to the buy price of electricity for the company. This scenario is subdivided in the two previously mentioned situations of avoiding the purchase of energy from the grid and avoiding burning biogas, to compare the results obtained between them. Although implementing a REC can lead to administrative and legal costs, and even permitting fees, there are currently several grants to help the realisation of REC in Portugal and the EU (*Fundo Ambiental, Ministério do Ambiente*, no date). As such, the costs and benefits of each of those will be ignored, and the only cost considered is the PV installation cost. The project is evaluated, from a previous study, in 398,238.46€. For every scenario, maintenance and other operational costs were arbitrarily positioned at 2% of the total investment cost.

To evaluate the costs and the results of each scenario, it is useful to apply economic indicators, as presented in section 2.3 . The selected indicators are the internal rate of return (IRR), NPV, and the already mentioned CRP. Below are presented the formulas for each of these financial indicators, as well as the formulas to calculate the annual cash-flow (C_{annual}), updated cash-flow ($C_{updated}$), and accumulated annual cash-flow ($C_{accumulated}$):

$$C_{annual} = AnnualProfit - Maintenance \tag{11}$$

$$C_{updated} = \frac{C_{annual}}{(1+u)^{year}} \tag{12}$$

$$C_{accumulated} = C_{annual}^{year-1} + C_{updated}^{year} \tag{13}$$

$$NPV = \sum_{x=0}^{X} \frac{C_x}{(1+r)^x} \tag{14}$$

$$0 = NPV = \sum_{x=0}^{X} \frac{C_x}{(1+IRR)^x} \tag{15}$$

$$CRP = \frac{\ln\left(\frac{C_{annual}}{(C_{annual}) - u * I_i}\right)}{\ln(1+u)} \tag{16}$$

, where u is the update rate, C_{annual}^{year-1} is the accumulated annual cash-flow of the previous year, $C_{updated}^{year}$ is the updated annual cash-flow of the current year, X is the total number of periods, x is a non-negative integer, C is the cash-flow, r is internal rate of return, and I_i is the initial investment. When equation 14 is solved for NPV equal to zero, as shown in equation 15, the value of the internal rate of return is the value of IRR. These indicators are capable of evaluating the potential and the risk of an investment, facilitating the comparison and the decision-making process.

5 Results and discussion

5.1 Optimization

5.1.1 Multi-objective simulations

The first simulation considered is a compromise between the two main objectives. The process began with the design of the main flowchart. The intended purpose of this flowchart was to sketch a model capable of producing significant economic savings, as well as limit the burnt biogas during the daily operations. The resulting flowchart is presented in Figure 17.

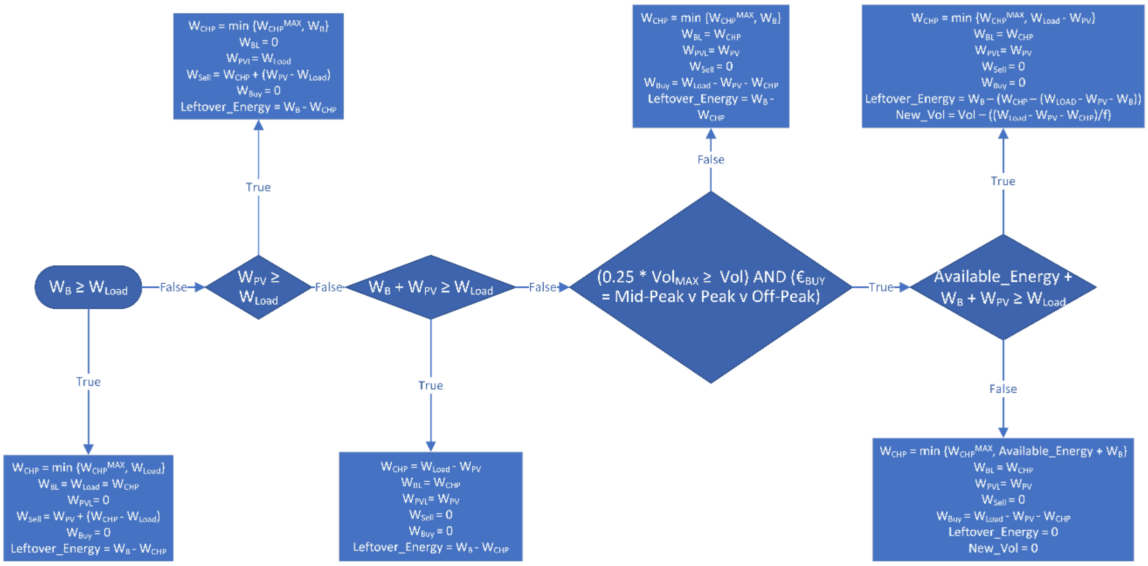


Figure 17 – Flowchart for multi-objective simulation

The decision process relies on five decision points. In each, a different set of criteria is evaluated, in order to achieve the desired target. The first decision point intends to assess if the biogas produced in the hour considered is sufficient to satisfy the energetic needs of the WWTP. Since biogas production is quantified in cubic meters per hour, the conversion factor is applied to convert the flowrate of biogas into expected production of electricity, as described in formula 17:

$$\dot{Q}_B * f = \dot{W}_B \qquad (17)$$

, where f is equal to 2.3 kWh/m^3, as stated in section 4.4. Afterwards, a sequence analyses if either the PV produced, or the sum of PV and biogas production can cover the electricity needs of the plant. After all of the current production possibilities are exhausted, the system must rely on its storage capacity. However, that step will be considered together with the current price to purchase electricity from the general grid. If the price is either peak or mid-peak, the two highest, the volume inside the gasometer will be utilized to supress the needs of the plant. If not, energy will be purchased to ensure that biogas reserves can be maintained for the higher priced hours. A lower safety threshold is established at 25% of the maximum capacity of the gasometer. This percentage will be kept to account for the peak and mid-peak periods when energy acquisition must be avoided at all costs. In this scenario, contemplated in the final decision point, all energy produced and stored will be used. Once the energy purchase price decreases, the system can re-enter the charging stage and replenish the stocks of biogas in the reservoir.

In addition to the main flowchart, a secondary flowchart was developed. The scheme shown on Figure 18 is dedicated to the leftover energy. This will be in charge of the response given to the amount of biogas being produced, in comparison to the biogas inside the gasometer and the portion utilized to produce electricity. When necessary, the torch will be activated to ensure the safety of the system.

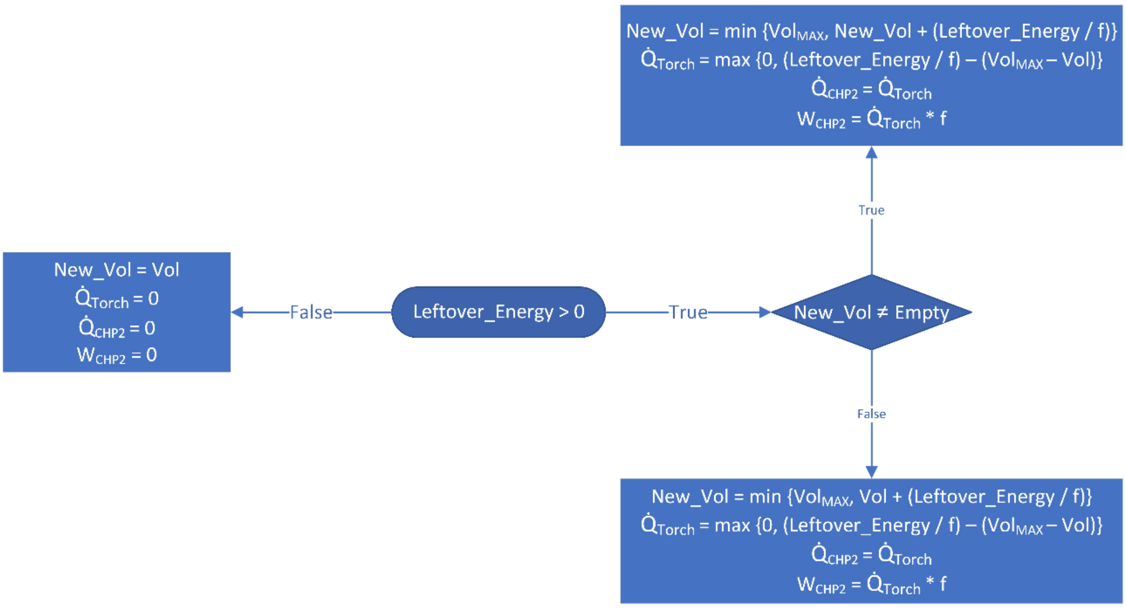


Figure 18 - Leftover energy flowchart

The required data is inserted into an Excel spreadsheet. With this flowchart as a starting point, the VBA code was written to incapsulate the conditions described. The VBA code can be analysed in full on Appendix B.1.

Deriving from the flowchart depicted in Figure 17, a parallel flowchart was developed. The main purpose of this variation was to create a model which preferred the usage of the stored biogas, instead of stacking until the closer to the superior limit. The adaptation is shown in Figure 19.

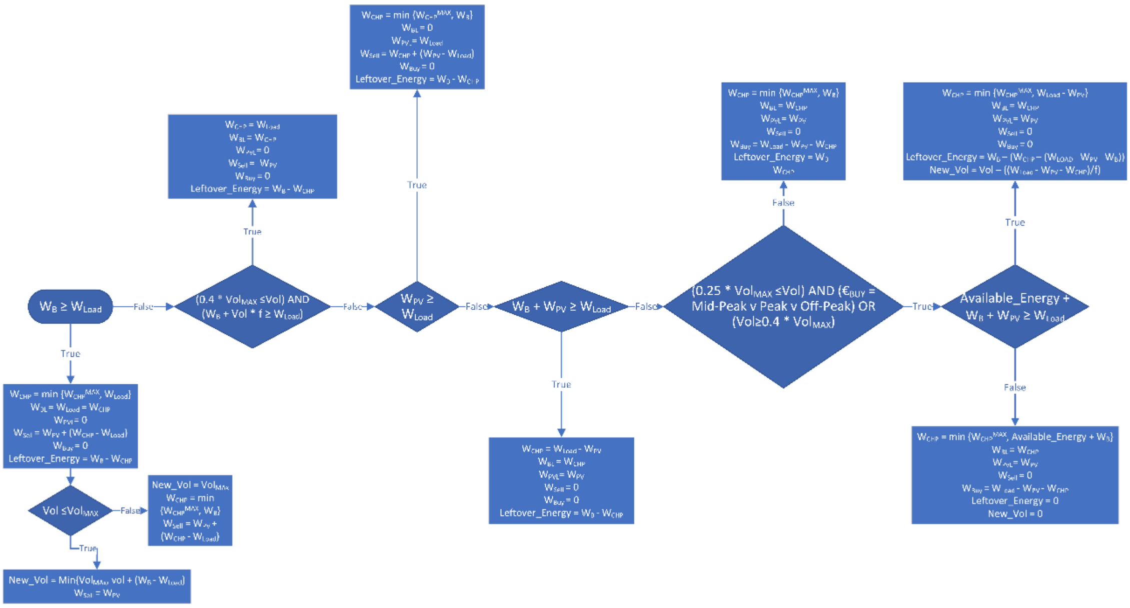


Figure 19 - Flowchart for multi-objective simulation, with preference for utilizing the stored biogas

Before assessing if the PV is sufficient to cover the energetic needs of the plant, the simulation will give preference to the stored biogas, if it possesses more than a defined plateau. In this case, the barrier was set at 40% of the maximum volume in the gasometer. Only if this condition is failed will the system resort to utilizing PV or the general electrical grid. The code utilized for this simulation can be found in full on Appendix B.2.

Both simulations utilized the 2023 hourly dataset for biogas and electricity needs of the WWTP. However, while the first simulation only used this dataset, the second simulation also considered the potential PV production for this time period. As such, the second simulation will naturally have more energy at their disposal. For the leftover energy, the flowchart of Figure 18 was maintained for both simulations' VBA code.

5.1.2 Simulation to minimize the bought electricity

The purpose of this simulation is to focus on only one of the objectives. In this case, the simulation's goal is to minimize the amount of energy purchased throughout the year, relegating the amount of burnt biogas to the role of consequence, rather than the one of a primary objective. For this simulation, a flowchart was designed with this in mind, as presented in Figure 20.

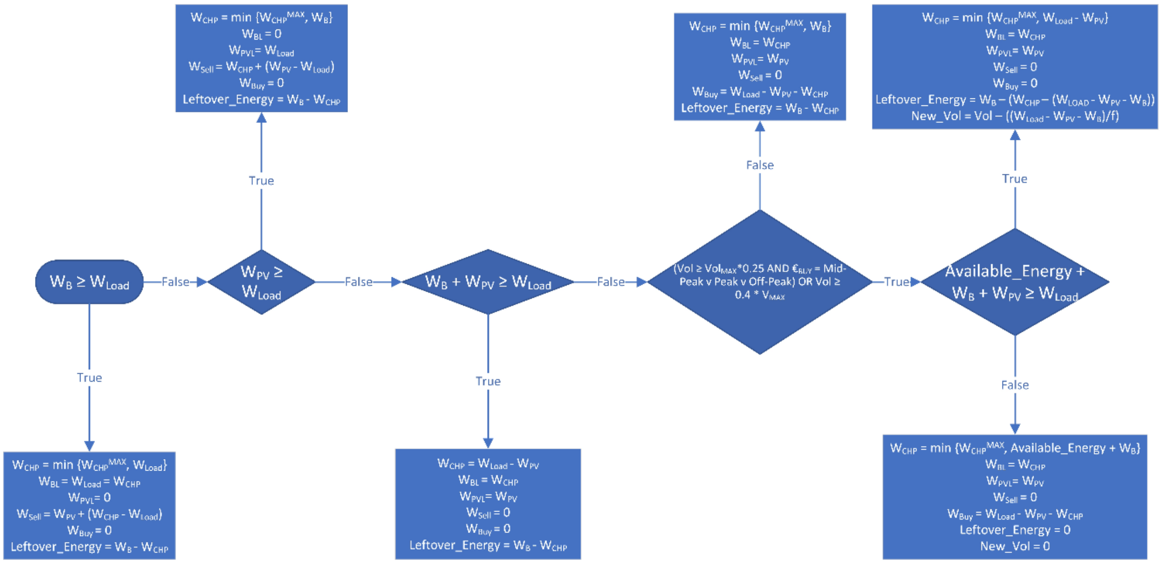


Figure 20 - Flowchart for purchase of electricity minimization simulation

When comparing to the flowcharts presented in section 5.1.1, the main difference resides in the opening of the criteria for utilizing the energy in stock inside the gasometer. The first three conditions remain the same, as does their respective outputs. In the final two conditions, electricity will be purchased if the volume is either below the minimum threshold of 25% of the maximum volume and if the price of electricity is the lowest possible throughout the day, or if no other option is available to satisfy the energetic needs of the WWTP. The full VBA code is available on Appendix B.3.

This simulation utilizes data for biogas, PV, and electricity needs of the WWTP from 2023. For the leftover energy, the flowchart shown in Figure 18 was utilized.

5.1.3 Simulation to minimize the burned biogas

The final simulation intended to mimic the previous one. It focuses just on one of the objectives, in this case, minimizing the total burned biogas throughout the entire year. The purchase of energy is left as a consequence of the remaining processes. For this simulation, the flowchart designed is presented on Figure 21.

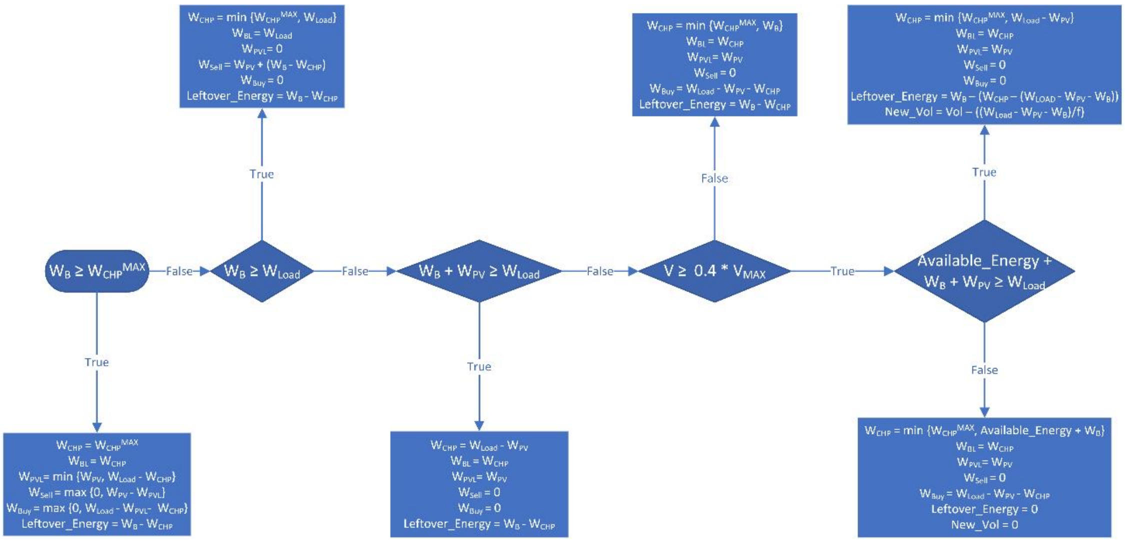


Figure 21 - Flowchart for burnt biogas minimization simulation

When comparing to the previously designed flowcharts, this one possesses the greatest number of changes. For starters, the first condition to be verified is no longer if the current production of biogas is enough to satisfy the energetic needs of the WWTP. In this scenario, the first analysed condition is if the current production of biogas is greater than the maximum capacity of the CHP. If that is verified, the CHP will start functioning at its maximum capacity, to minimize the amount of biogas being stored. Reserves of biogas are kept low throughout the scheme, to leave room for manoeuvre in the event of high production of biogas during a continuous period of time.

Since minimizing the cost of purchased energy is not one of the objectives considered in this scenario, conditions that related to it are removed from the flowchart. In decision point 4, only the amount of stored biogas is considered to decide, in opposition to the flowcharts shown in Figure 17, Figure 19, and Figure 20.

Contrary to previous approaches, the leftover energy also suffered adaptations, as shown in Figure 22. This flowchart will search for possibilities to increment production of CHP. Burning biogas will only be a last resort option, if all of the other options are of the table. As such, this flowchart can directly impact and change the outputs decided by the previous one. In the case of an increase in biogas levels, the CHP can be put on maximum power to attempt to transform as much biogas into electricity as possible.

For this simulation, data from 2023 for both biogas, PV, and electricity needs of the WWTP were utilized. The VBA code which represents the flowcharts presented can be accessed in full on Appendix B.4.

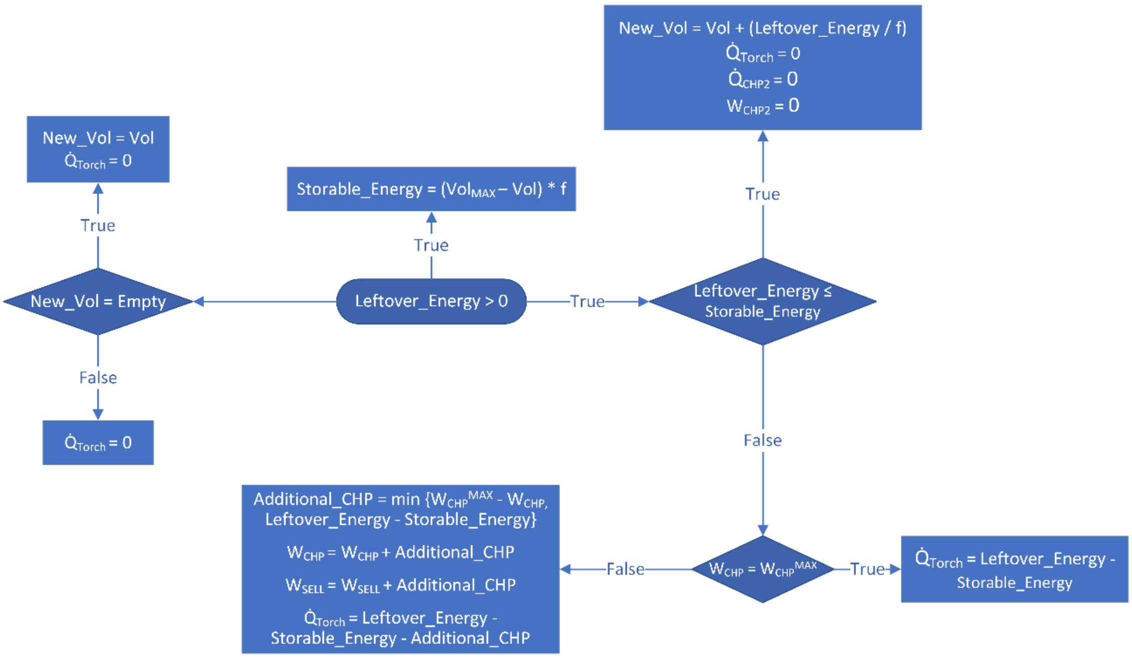


Figure 22 - Leftover energy flowchart for burnt biogas minimization simulation

5.1.4 Discussion and analysis of the results

In this section, the results obtained from the simulations will be presented. These will be analysed based on seven indicators: total electricity purchased, total electricity donated to the REC, total biogas burned, total cost of purchased electricity, total savings from energy donated to the REC, wasted biogas ratio, and self-sufficiency ratio. These metrics should help analyse and compare the different simulations, in spite of the different base conditions of each one. The results obtained are summarized in Table 2.

Table 2 - Summary of the results obtained for the simulations

Renewable energy sources considered	**Simulation 1: Biogas**	**Simulation 2: Biogas + PV (in favour of using stored biogas)**	**Simulation 3: Biogas + PV (avoids the purchase of electricity)**	**Simulation 4: Biogas + PV (avoids burning biogas)**
Total electricity purchased	1,156,857.47 kWh	377,542.97 kWh	23,818.30 kWh	392,080.73 kWh
Total electricity donated to REC	0 kWh	625,904.95 kWh	1,393,698.91 kWh	1,452,189.90 kWh
Total biogas burned	0 m^3	0 m^3	416,675.14 m^3	0 m^3
Total cost of purchased electricity	122,624.88 €	38,785.14 €	2,446.14 €	40,430.02 €
Total savings of energy donated to REC	0 €	70,348.76 €	156,049.90 €	162,026.75 €
Wasted biogas ratio	0.00%	0.00%	25.19%	0.00%
Self-sufficiency ratio	74.00%	91.52%	99.46%	91.19%

As can be inferred from the results, the output suffers substantial changes from the presence of PV production and depending on the approach taken for simulation. In all of the scenarios, energy purchasing is occurring. However, whilst in the first, second, and fourth simulations energy purchasing is unavoidable, in the third scenario it is likely that the purchase of external electricity from the general grid could be avoided. In fact, this is the only simulation that achieves above 99% of SSR. According to data from 2021 until the beginning of 2024, shown in Figure 23, the WWTP was unable to achieve SSR above the 72%. When comparing to the results obtained in these simulations, it shows a solid improvement derived from the optimization mechanisms. Even for the first simulation, which mimics the conditions of the time period, a 74% SSR combined with the absence of burned biogas translates into a superior result than the ones previously achieved.

The results rendered by the last simulation are worse than the ones obtained by the second simulation, regardless of the analysed metrics. Thus, it is safe to assume that, with the conditions described, this is not a valid option for simulation and one of the other routes should be taken into consideration.

The approach that avoids the purchase of electricity from the general grid is also the one that wastes the most biogas. The remaining simulations achieved zero wasted biogas.

Although the first simulation, that only considered biogas production, achieved solid results, PV implementation is shown to have a significant positive impact in the economic aspect of the WWTP. All three scenarios managed to donate a significant amount of energy towards the REC while bridging the existing gaps in the WWTP energetic scheme.

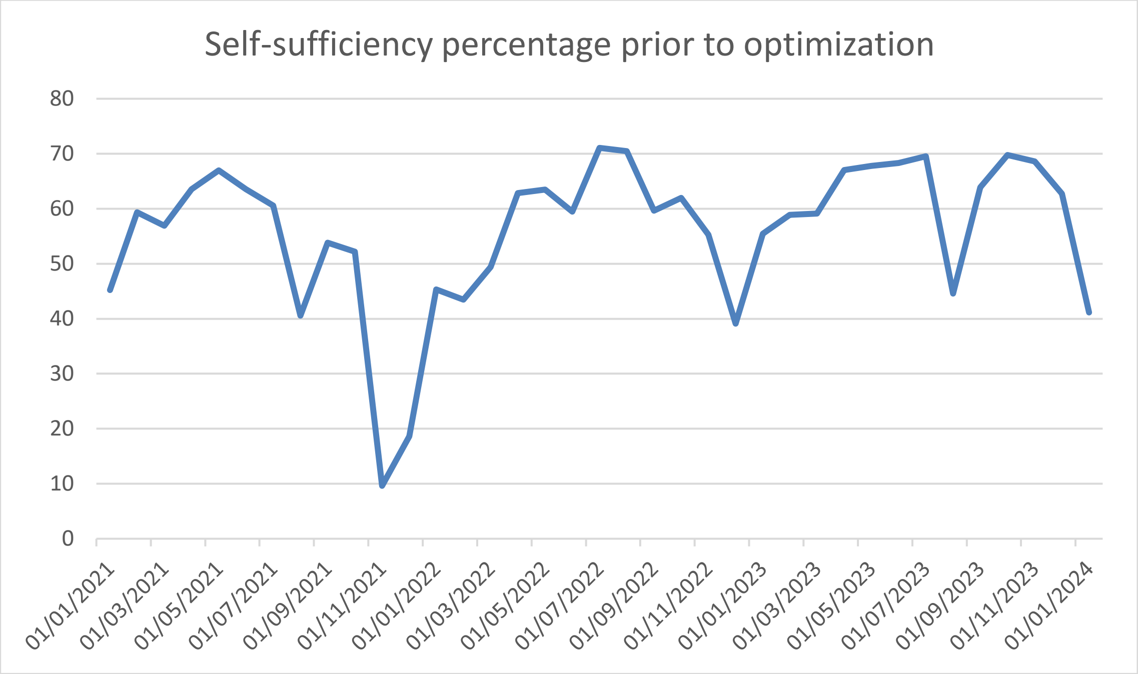


Figure 23 - Self-sufficiency percentage prior to optimization

5.2 Economic analysis

5.2.1 PV viability

Due to the high biogas production, especially when compared to the energetic necessities of the WWTP, an economic analysis of the investment in PV technology was carried out. For the initial investment, the value considered of 398,238.46€ is based on a previous study carried out by the company. The maintenance and update rate are placed at 2% and 7% respectively. No residual value of the investment was considered for any of the propositions.

In this study, three cases were considered. The first case is referred to the results obtained in the simulation 4, in Table 2, and the second case is referred to simulation 3. In these, a majority of the produced electricity in the plant is forwarded towards the REC, deeming these to be the cases with the highest potential for investment. The third case refers to simulation 2 of the aforementioned table. This scenario only donates half of the electricity of the other two scenarios; thus, it is predicted to have a smaller potential for investment than the remaining cases. The results for the three cases are compiled in Table 3.

Table 3 - Excess energy produced is sent to a REC

Cases	**Case 1: burning biogas is avoided**	**Case 2: buying energy is avoided**	**Case 3: favours the usage of stored biogas**
Initial investment	398,238.46 €	398,238.46 €	398,238.46 €
Annual Profit (constant)	162,026.75 €	156,049.90 €	70,348.76 €
Update rate	7%	7%	7%
Residual value of investment	0	0	0
Maintenance	7,964.77 €	7,964.77 €	7,964.77 €
NPV	1,513,523 €	1,439,356 €	375,887 €
IRR	38.68 %	37.18 %	15.45 %
CRP	2.950 years	3.083 years	8.752 years

As predicted, the first and second cases have the highest NPV and IRR and the lowest CRP. Comparing to the remaining case, these are the best investment possibilities. Not only that but, considering the investment itself, with only 3 years to recover the initially invested capital, it is a highly advantageous investment possibility in both scenarios. The remaining case has a lower NPV and IRR, making it a riskier investment overall.

However, donating the excess electricity towards a REC is not the only possibility for the company. It can also sell it to the grid. Since, currently, the WWTP does not have a contractualised value for selling the excess energy produced in their installations, it is resorted to a sensitivity analysis for the selling price of electricity. As such, it is selected the worst case out of the previously presented, which is the case where the usage of stored biogas is favoured. If the results show the possibility for investment with this scenario, then it is safe to conclude that the remaining scenarios will also be a solid investment. For this scenario, four electricity selling prices were analysed, and the results are compiled in Table 4.

Table 4 - Excess energy produced is sold to the grid; Stored biogas usage is favoured

Selling price of electricity to the grid	**0.10 €/kWh**	**0.15 €/kWh**	**0.20 €/kWh**	**0.25 €/kWh**
Initial investment	398,238.46 €	398,238.46 €	398,238.46 €	398,238.46 €
Annual Profit (constant)	62,590.50 €	93,885.74 €	125,180.99 €	156,476.24 €
Update rate	7%	7%	7%	7%
Residual value of investment	0	0	0	0
Maintenance	7,964.77 €	7,964.77 €	7,964.77 €	7,964.77 €
NPV	279,614 €	667,958 €	1,056,302 €	1,444,646 €
IRR	13.40 %	21.51 %	29.42 %	37.29 %
CRP	10.553 years	5.797 years	4.014 years	3.073 years

Results show that, from 0.15 €/kWh, the investment is more beneficial than providing the same electricity to the REC. The investment increases in upsides as the sell price increases, with a rise in annual profits, NPV, and IRR, and decrease in CRP. However, it also shows that the viability of this choice is heavily dependent on the contractualised conditions and the determined selling price for the electricity.

Overall, the installation of a PV system in the WWTP has potential to be a solid investment opportunity. Nonetheless, it requires solid management of the energy sources to be viable, since it is necessary to utilize biogas to mainly satisfy the necessities of the plant, in order to allow for a more beneficial financial upside.

5.2.2 Second CHP viability

The second investment opportunity presented comes as a consequence of the defined objectives for the optimization process. Although some of the simulations managed to minimize the burned biogas, one alternative for the excess energy produced would be the implementation of a second CHP unit. This unit would be smaller than the one currently in place, to accommodate the current necessities of the WWTP.

Since only two of the simulations in Table 2 presented a flowrate of biogas being burned, only two scenarios were accounted for in this analysis. The first scenario refers to the first simulation performed. With an excess biogas production of only 1454.75 m^3, the size of the required CHP unit is very small. As stated in section 4.5, the value of a CHP unit is variable, according to the desired power output. As such, for this case, an initial investment of 200,000€ was considered. The results are shown in Table 5.

Table 5 - Implementation of a second CHP unit; biogas data

Case 1	**Value**
Initial investment	200,000.00 €
Annual Profit (constant)	6,368.93 €
Update rate	7%
Residual value of investment	0
Maintenance	4,000.00 €
NPV	-170,604 €
IRR	-5.70%
CRP	Impossible

The results obtained show that the investment, in these conditions, is impossible. The initial investment is overwhelmingly high when compared to the potential annual profits derived from this investment. The NPV and IRR indicators are both negative, meaning that the cash-flows are not enough to cover the initial investment cost.

The second investment opportunity appears in simulation 3, which has a total yearly burned biogas flowrate of 416,675.14 m^3. On the one hand, the higher amount of biogas available for the second CHP unit means it can produce more and generate more electricity, resulting in a substantially larger annual profit. However, it comes at a cost. The initial investment must match the increase in flowrate, thus making the cost of the CHP more elevated. For this scenario, an initial investment value of 600,000€ is selected. The results are compiled in Table 6.

Table 6 - Implementation of a second CHP unit; Biogas and PV data; Buying energy is avoided

Case 2	**Value**
Initial investment	600,000€
Annual Profit (constant)	104,650.94 €
Update rate	7%
Residual value of investment	0
Maintenance	12,000.00 €
NPV	549,709 €
IRR	15.22 %
CRP	8.925 years

Results show that, unlike the previously proposed investment scenario, this has the potential to generate profit. It is estimated that, within 8.925 years, the initial investment will be recuperated. The IRR of 15.22% suggests that this is an attractive investment opportunity, with a solid risk-reward trade-off.

With the corresponding model for optimization of the energetic systems of the WWTP, the implementation of a secondary CHP unit shows potential to be a successful way to mitigate losses of biogas via burning. Additionally, it will render an increase in production output of energy, which, combined with the implementation of a REC or by selling the excess energy to the general grid, can not only result in this WWTP becoming fully self-sufficient, but generate profit from the excess energy or even help other infrastructures become self-sufficient.

6 Conclusion

In this work, a simulation mechanism was developed for the optimization of energy resources in a MES. In section 2, an in-depth review of the existing modelling systems was conducted. It also delved into the legislative conditionings, as well as the types of economic analysis performed in these scenarios. In addition, section 3 presented the most recent applications for both solar energy and biogas, with a particular emphasis on the latest WWTP purposes.

The developed procedures were tested and applied to the case of the WWTP of *Gaia Litoral*, as presented in section 4.1. The WWTP showed good characteristics to become self-sustainable and more ecologically efficient. It has production of biogas, through anaerobic digestion, and PV production. Often the biogas production alone is sufficient to satisfy the energetic needs of the plant, thus leading to the desired objectives: minimize the biogas burned in the torch, reduce the necessity to purchase electricity from the general grid, and, ultimately, achieve self-sufficiency. The flowchart approach was selected in section 4.2 as the preferred model, due to its simplicity, being easy to understand and manipulate, and flexible. It allows for manoeuvrability in defining the objectives for optimization and the conditions that will limit them. This approach was developed in section 5.1 and was successfully implemented.

Four optimisation scenarios were designed, and its results were presented in section 5.1.4. Two of the models were designed with the intention of achieving a compromise between reducing the burnt biogas flowrate and the desired economic savings. One of the models only utilized data given by the company, in the form of biogas production data and overall WWTP load necessities. The second model added to the first one the historical irradiance data retrieved from the Solcast API, which was used with the formulas on section 4.3 to estimate the PV production. The remaining two scenarios were focused on achieving the best possible results on a singular objective. Both used all of the datasets available. The first one focused on minimising the amount of burned biogas, while the second one aimed towards reducing the amount of energy purchased and, subsequently, the overall costs.

Each scenario showed superior results to those prior to optimization. Out of the four cases, two managed to avoided burning biogas altogether for the entire year. In spite of none of the simulations being able to avoid purchasing energy, the results were still substantially better than the ones before the optimization. The case dedicated to minimising the purchase of electricity managed to purchase just 23,818.30 kWh of energy over the course of a year, which is equivalent to an estimated 2,446.14 €. For the third objective present, which was analysed as a byproduct of the other two, self-sustainability suffered a tremendous improvement. After the introduction of the energy optimisation system, the self-sustainability ratio increased from 70% to over 91% in all the scenarios analysed that considered biogas and PV production, with scenarios focused on avoiding the purchase of electricity from the grid achieving a 99.46% ratio.

The application of a secondary cogeneration unit was explored, to reduce the amount of burnt biogas in low-purchase scenarios. Results showed that the application of a second cogeneration unit can be profitable, if the wasted biogas is close to 25% of the total production. For lower amounts of biogas, the profit does not compensate for the initial investment

Lastly, the cost-effectiveness of the implementation of the photovoltaic system was also analysed, due to the excessive amount of exceeding energy derived from this source of energy. Two solutions were examined: the first one showed that establishing a renewable energy community with neighbouring facilities is a viable alternative to utilize the excess of produced electricity, with the internal rate of return oscillating between 38.68% and 15.45%, depending on the simulation scenario; the second analysis consisted of a sensitivity analysis of the selling price of electricity. It utilized the scenario which yielded the worst result on the previous analysis. It determined that, for selling prices higher than 0.15 €/kWh, it can be a viable option to sell the electricity back to the grid, even though it does not achieve the same economic benefits as the community approach.

6.1 Future work

In the following, suggestions for future work possibilities are presented.

1. Test the application of different modelling approaches. With the predominance of AI and ML, new applications can appear and result in better and optimal solutions.
2. Test the capabilities of the model for lower time-step applications (fifteen minutes, five minutes, and so on).
3. Implement the model in a real-time capacity. With the use of Solcast API for PV estimation, it requires the implementation of real-time predictions for the energetic load of the WWTP and the expected biogas intake for the foreseeable future.
4. Incorporate the heat into the calculations of the CHP. In this case study, the heat produced by the CHP was not considered, due to it not being the focus of the work.

However, the incorporation of heat can lead to different variables to be analysed and different constraints.

5. In the investment applications, other combinations can be tested besides the ones analysed. This will explore different possibilities and applications for the electricity produced. In addition, considering varying annual profits instead of constant annual profits can also increase the authenticity.

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Appendix A - Review of relevant modelling studies in literature

Models	Case study	Key findings	Reference
Stochastic Model Distributionally Robust Optimization (DRO)	Comparison of a stochastic model to a min-max approach, solvable through a linear solver. Comparison of DRO-L (symmetrical variation ranges) and DRO-U (asymmetrical) to stochastic solutions.	DRO investment strategies are quite stable and yield more diverse investments than stochastic models. Robust solution yielded the lowest average investment cost, although it had the highest standard deviation in operation costs and fails to keep up with demand variability in the heating sector. All models had acceptable feasibility. Robust and worst-case scenario had the highest. These solutions provide a good trade-off between cost, variability, distribution independence and out-of-sample independence, making DRO solution the recommended strategy for this case.	Guevara *et al.* (2020)
Deep Neural Networks (DNN) Random Forest (RF)	Five different cases, with various levels, focuses of optimization, and time frames. The objective of optimization consisted in minimizing the total cost of operation over 24 hours in a building. Case 1: conventional; cooling tower (CT); integrated; optimized number of CT; optimization of CT operation (real conditions). Case 2: conventional; integrated; optimization;	DNN was the most accurate model, followed by RF. Epsilon constrained differential evolution is proposed to determine daily operating schedules. DNN proposed to forecast optimal operating conditions. The proposed optimization method, case 3, reduced operating costs 17.4% and decreased primary energy consumption when	Ikeda and Nagai (2021)

	optimization (CHP extended to 24h). Case 3: optimization; integrated; optimization; optimization. Case 4: optimization; integrated; minimum; rate speed. Case 5: optimization; individual; minimum; rate speed.	compared to cases 1 and 2. Also resulted in a 10.2% reduction in daily operating costs and 8.0% reduction in primary energy consumption compared to case 4. Case 3 had a 16.8% reduction in daily operating costs and 12.9% reduction in primary energy consumption, comparing to case 5.	
Artificial Neural Networks (ANN) ALAMO modelling tool	ANN were trained to predict the total revenue and number of startups as a function of generator bid parameters and compared to ALAMO as a baseline. Case study: uses the Rankine Cycle as the representative supercritical thermal steam generator and calculates the capital cost, operating cost, heat rate, and cycle efficiency as a function of the operating capacity. Two approaches: use of market-based surrogates and a price-taker approach.	Results show the limitation of the self-schedule and price taker assumptions. ALAMO values of R^2 (regression coefficient) were 0.825 and 0.419 while the R^2 of the ANN were greater than 0.99 in both. Use of market-based surrogates in optimization is computationally efficient (can be solved in seconds) and provides verifiable design solutions, capturing dynamic effects that the price-taker approach cannot consider. Price-taker approach can take longer to be solved, depending on the number of scenarios. Price-taker performs well at low marginal costs but over-predicts revenue and under-predicts operating costs.	Jalving *et al.* (2023)
Mathematical model	Energy optimization of the largest WWTP in Italy. Use of empirical formulas, proportional-integral controllers, among other, to simulate the WWTP processes.	Results demonstrate the promising potential of significant reductions in energy consumption, while maintaining effluent quality, through operational changes.	Borzooei *et al.* (2020)

	Limited energy audit data at disposal. Use of two performance assessment criteria: effluent quality and energy saved.		
Monte Carlo simulation (MCS) Discrete Event Simulation (DES) Predictive algorithms: ERIM-P (energy resources intelligent management - predictor) and ERIM-RT (energy resources intelligent management – real-time)	Objectives: minimize CO_2 emissions, achieve net zero between consumed and produced energy, and minimize energy costs in a singular building. A sub-model predicts RES availability, while another one simulates the manufacturing plant. Four scenarios presented, with different PV characteristics. ERIM-P forecasts hourly electrical energy requirements and self-production of RES based on weather predictions. ERIM-RT acts on current day, considering real-time DES and weather. ERIM-P and ERIM-RT are combined using MCS.	ERIM-RT model improves energy performance and reduces error, CO_2 emissions, and energy costs, especially in scenarios with high deviations between prediction and actual profiles. ERIM-RT improves ERIM-P's performances by providing accurate hourly demand profiles and lower costs for energy used. Provides benefits in the capacity to describe the behaviour of complex systems, but unpredictable events can create deviations. Statistical validation tests showed that the DES simulation model was accurate and reliable; the difference between it and actual consumption being 3%. Cost reduction oscillated between 230€ and 900€ per day, depending on the scenario analysed. CO_2 emissions reduction was situated between 390 kg and 1038 kg per day, depending on the scenario analysed.	Cassettari *et al.* (2017)
Greedy Algorithm: piece by piece solution	GAN algorithm was applied to the selected data, while the remaining were used as comparative cases for the overall optimization of a large industrial park.	For users with a regular power consumption, the simpler averaging strategies are highly competitive for these applications.	Gao, Li and Hong (2021)

Genetic Algorithm (GA): inspired by natural evolution Generative Adversarial Network (GAN): machine learning Deep Deterministic Policy Gradient (DDPG): uses deep reinforcement learning	Prediction of electricity load and PV power generation for the following day. The predicted reference data were outputted by GAN and simple averaging and compared with the actual output. Option for the users to choose between day-ahead or real-time trading methods. Step size of one hour.	All methods can optimize operating cost of a system. DDPG is easier to obtain an optimal solution than Greedy and GA. Greedy wastes energy. The final proposed solution involved GAN prediction and DDPG scheduling to optimize power consumption for users who have power generation devices. DDPG can reduce operating costs by 35.9% in the given scenario. The Greedy method stores a lot of energy in batteries, wasting it because its main priority is to satisfy a possible future energy shortage. DDPG has a less stable algorithm than GA.	
Actual Engineering Models (AEMs) Artificial Neural Networks (ANN) Hybrid Optimization Algorithm (HOA)	AEMs are responsible for optimizing the energy system on an hourly basis. Creation of two paths, composed of partially different blocks; one path is responsible for optimizing the energy system while the other evaluates the objective function values and updates the population. Black box model is a surrogate model, used to reduce computational time by mapping the decision space variables into the objective space. ANNs were trained with Levenberg-Marquardt back propagation. These two are combined to form a HOA, where the surrogate model is used to	Best performance was achieved with shallow network with two layers and fifty neurons per layer. When grid integrations are below 10%, the Pareto front obtained using the surrogate model shows a significant increase in NPV compared to AEM. Solar PV capacity slightly higher in the Pareto solutions obtained with AEM. Deviations in wind turbine, ICG and battery bank capacities. Surrogate models are more reliant on wind turbine than solar PV, contrary to AEM.	Perera *et al.* (2019)

	generate the initial Pareto front and AEM to refine it. 448,000 samples were used for initial model training, 192,000 samples for validation, and 640,000 samples for testing the model.		
Deep Reinforcement Learning (DRL) Deep Neural Networks (DNN) Deep Deterministic Policy Gradient (DDPG) Twin delayed deep deterministic policy gradient (TD3)	Singular building. Hybrid system, combining PV, storage, and general grid. Requires a large amount of data. DRL to solve sequential decision problems. DNN for estimating cumulative rewards.	DRL was able to optimize the operation, including equipment scheduling and RES. Achieved goal of off-grid operation and battery safe operation. The DDPG and TD3 algorithms experienced two stages of learning and convergence; TD3 outperformed during most of training time. In testing, cumulative reward show the same trend as training, but there's an initial uncertainty period. Both methods outperformed rule-based control. DDPG achieved the worst results in terms of off-grid optimization. TD3 performed slightly better than the baseline control model. TD3 and DDPG had almost no need to sell energy to the grid.	Gao *et al.* (2022)
Deep Neural Networks (DNN)	DNN functions as a surrogate model to data generated by a simulator and adapt the optimization problem to converge to the optimal operating conditions for a real plant, via real-time optimization. The methylene diphenyl diisocyanates production process can be simulated	This approach is not viable for large-scale processes, becoming highly time consuming. Use of a modifier adaptation resulted in the problem being iteratively updated by correction of terms, afterwards it converged to plant optimum.	Ehlhardt *et al.* (2023)

	by an operating training simulator, used to predict measurements from the real plant. Use of a two-step approach to avoid mismatch.	When enough data points are available, the objective function starts to converge, without all constraints being fulfilled. The constraint functions of the rigorous model and the operator training simulator are mismatched. Successful implementation of an iterative real-time optimization model.	
Linear Regression Non-linear Regression Neural Network Regression Recurrent Neural Network Long Short-term Memorie (LSTM)	Different algorithms used in a test bench for energy forecasting. The test model included simulations for PV, wind, and hydropower energy.	This test bench can be implemented with a very low cost when compared to existing solutions. For the test model, the solutions that achieved the best results was LSTM.	Laayati *et al.* (2022)
Distribution Energy Resource Management Systems (DERMS)	Study executed on distribution grids with high penetration renewable distributed energy resources. Focuses on addressing the technical problems caused by the high variability of RES and estimate the flexibility in real-time. Utility DERMs is an intelligent software platform for the optimal management of medium to large scale DERs. Consists of several modules integrated into a single solution and must be fully-grid aware, have accurate network model, ingest all	A state-of-the-art DERMS solution can provide the required capabilities to safely overcome the incoming challenges. Most renewable DERs are connected to the grid via smart inverters, which can be controlled through utility DERMs. Utility DERMs can provide the same services as baseload power plants but in a more rapid, efficient, and pollution-free way. It also provides both real-time measurements and an accurate network model to distribution utilities.	Strezoski and Stefani (2021)

	available measurements from the field, and integrate with weather providers.	Utility DERMs predicts and proactively mitigates potential grid violations with great precision.	
Long Short-term Memorie (LSTM)	Proposed ML model that can be used to develop high-level learning in smart cities and maintain system performance. Proposed LSTM model to forecast electricity prices and demands using real market data.	Both models were able to address the challenges proposed and achieve the main objectives. Concerns for cyber-security.	Ullah *et al.* (2020)
Deep Learning (DL) Artificial Neural Network (ANN) Deep Neural Networks (DNN) Long Short-term Memorie (LSTM) Deep Belief Network (DBN)	LSTM is used to predict a new initial value. DNN is used to add new layers to the forecast. Use of multiple ANN architectures: multilayer perception, LSTM, deep belief network, auto-LSTM, and activation functions. A tanh activation function was used in all layers except in the output layer (Rectified Linear Unit was used). A physical photovoltaic forecasting model was used as a reference. It doesn't use any part of the data set, relying only on coordinates and angles to start. Also uses parameters such as temperature and the direct and diffuse solar radiation. Use of a Clear Sky filter: estimates terrestrial solar radiation of the sun with a cloudless sky, while also preventing nighttime forecasting (if clear sky indicates a null value, then the physical photovoltaic model is also set to zero). Used dataset of a German solar farm.	DL has been used to forecast regenerative energy sources such as wind power. In this case, ANN and DNN are introduced, successfully, for forecasting of solar power output. Usage of a min-max normalization allows for a comparison without having to consider the size of the PV facilities. All models had to predict the day-ahead forecast. All analysed ANN and DNN models outperformed the Physical model. The best DNN is Auto-LSTM. DBN also shows error values on par with Auto-LSTM, the slightly increased forecast error is extrapolated to be due to the existence of an attached linear ANN layer instead of an LSTM layer. Results also show that some facilities might be easier to predict than others due to unpredictable characteristics. ANN and DNN models perform better than	Gensler *et al.* (2016)

	Comparison between the data set and the physical model is enabled by the usage of a min-max normalization in the measured power output variable. All models had to predict the day-ahead forecast.	physical, due to the fact that the aforementioned models take extreme weather situations into consideration.	
Deep Neural Networks (DNN)	Prediction of total daily incoming solar radiation. Use of Numerical Weather Prediction patterns to provide forecasts for a geographical area, by taking advantage of DNNs capabilities of dealing with bidimensional problems.	Extensive use of convolutional layers proved to be a key factor. Optimal set: first two convolutional layers with 150-channel outputs, two fully connected 400-unit layers, dropout coefficient of 0.2, mini-batch size of 150, and starting learning rate of 0.3. Support Vector Machine (SVM) required training each station individually, while DNN allows for simultaneous training. Whilst DNN is very powerful and yields better results than classic models, it is very costly to setup and train. DNN can be quite robust and improve the accuracy of singular networks. Use of parallelization is recommended to overcome high cost of training and model selection difficulties.	Díaz–Vico *et al.* (2017)
Probabilistic Methods	Analysis of two cases: a small-scale electrical network and a large-scale electrical network. MCS used as a base to compare results obtain by the Point Estimate Method (PEM). Case 1: In the PEM, 33 input random variables	PEM overcomes existing difficulties associated with the lack of perfect knowledge, achieving solid results and keeping computing time low. PEM renders good results when compared with MCS, both for the mean	Khorsand and Seifi (2018)

	were used. The number of estimations needed to obtain a solution were 66 or 67 (2m or 2m+1). Case 2: MCS with 7000 samples; PEM with 53 random input variables and a number of estimations of 106 or 107 (2m or 2m+1).	and the standard deviation. 2m+1 has a much smaller error than 2m scheme, making it able to conclude that 2m+1 renders the best results out of these three options. 2m+1 is also the faster to compute out of the three options (651 vs 89 vs 86 seconds).	
Diagonal Recurrent Wavelet Neural Networks (DRWNN)	DRWNN is based on the combination of recurrent neural networks with a wavelet one (activation function) plus fuzzy technology (input vector for cloud cover). Forecast of hourly and daily global irradiance. Back Propagation Neural Networks (BPNN) are used as a benchmark for this study.	The model is effective in providing higher forecast accuracy and generalization. According to the correlation coefficients obtained, to forecast hourly global irradiance for the next day, the records that are 14, 15, 28, and 29 hours before the hour to be forecasted are justifiable to be selected. The forecast results by the DRWNN coincide with the real records to a satisfactory extent, whilst the forecasts via BPNN do not achieve such results.	Cao and Lin (2008)
Support Vector Machine (SVM) Feedforward Neural Network (FNN) Deep Learning (DL): Long Short-term Memorie (LSTM)	Test the prediction accuracy of solar irradiance by SVM, FNN, and LSTM, due to these being the most widely used methods for forecasting in existing literature. LSTM was introduced to overcome the vanishing or exploding gradient problem.	LSTM achieved the best performance overall, followed by SVR and FNN, respectively. SVR and FNN presented lower accuracy and more bias error than LSTM.	Alzahrani *et al.* (2017)
Artificial Neural Networks (ANN) Support Vector Machine (SVM)	All models were trained with acquired datasets and relationships were constructed between inputs and outputs.	Good accuracy showed by the three models. However, ANN outperformed the remaining models.	Theocharides *et al.* (2018)

Regression Trees (RT) Persistence Model (PM) Feedforward Neural Network (FNN)	Intended to predict the power output for a PV system. The PM was used as a baseline comparison for the results obtained with the remaining models.	PM only showed good results for consecutive clear sky days. FFNN model is more accurate than SVM and RT. These two can be considered equivalent for this case.	
GPS-X modelling tool	Use of GPS-X to model WWTP. Two types of performance assessment criteria: effluent quality-based and energy-based.	Dynamic simulation showed that Solid Retention Time (SRT) of 25 days was the optimal operational condition for effluent quality and energy consumption. The minimum consumption of energy possible was obtained for SRT equal to 10 days. Prior to optimization, the WWTP would consume 0.3 kWh for treating 1 m^3 of wastewater. However, after the selected optimization was implemented, the consumed energy was reduced to 0.28 kWh/m^3 of wastewater.	Borzooei *et al.* (2019)
System-of-Systems (SoS) Multi-Criteria Analysis (MCA)	Presents a holistic methodological framework for evaluating integrated energy systems towards achieving the energy trilemma objectives: decarbonisation, acceptability, and security. The proposed framework combines a system-of-systems approach for systems analysis with an indicator-based approach using multi-criteria analysis. Uses a System-of-Systems (SoS) approach for system analysis, and an indicator-	This paper argues the need for a new evaluation framework that can holistically assess the performance of integrated energy systems. It has been validated using expert elicitation and is being applied to a case study to test its applicability. Six identified characteristics to evaluate the performance of IES: multidimensional, multi-vectoral, systemic, futuristic, systematic, and applicable.	Berjawi *et al.* (2021)

	based approach using Multi-Criteria Analysis (MCA) to evaluate integrated energy systems.		
Mathematical Model	Evaluates the performance of the most recent designs for energy generation by means of renewable energy sources, when operated as a cogeneration system. Framework for energy price estimation based on four different prosumers roles. The authors implemented a cost minimization problem for a microgrid network (PV panels, CHP, and local heating units).	The proposed model was validated in the microgrid system, with six houses acting as prosumers. The results showed that the integration of CHP system with solar panels could reduce the cost of microgrid system by 6.05%. Also contemplated three different scheduling strategies.	Bagherian and Mehranzamir (2020)
Segmented integral linearisation	Use of conditional value-at-risk method with segmented integral linearisation. Case 1: no dynamic characteristics Case 2: only dynamic characteristics of the heat network Case 3: only dynamic characteristics of the gas network Case 4: both dynamic characteristics. Constraints applied to power balance, generation capacity, ramping rates, transmission flows, wind power reserve, CHP, heat load, etc., that are meant to capture dynamic properties and make IES operation more practical.	Results confirmed the effectiveness. Dynamic characteristics of the heat-gas networks can be used for storage to increase the flexibility of the IES and accommodate more uncertain wind power.	Chen *et al.* (2020)
Mathematical Model	Smart grid with RES and CHP on the university of Genoa campus. Two CHP, two boilers (natural gas), thermal storage (3000 L), absorption chiller (70 kWth), three concentrated solar power units, electrical	Results showed that the smart microgrid can successfully determine economic and environmental advantages if operated under an optimized strategy. Hence, the model	Bracco *et al.* (2014)

	storage, PV field, and two recharging stations for EV's. Objective: minimize microgrid's daily operational costs. Seven main constraints applied. Mathematical model's main inputs were thermal load profile, electrical load profile, technical performance data of gas turbines and boilers, ambient conditions, and economic data (purchasing prices and maintenance costs)	presented is essential to guarantee efficiency.	

Appendix B – VBA code

In this appendix, the utilized VBA code is presented. For it to function, the following steps must be verified:

1. The name of the worksheet must match the name present in the code line “`Set ws = ThisWorkbook.Sheets("Simulation_2023_Hourly")`”.
2. The columns in the worksheet must match the organization followed in the code.

Appendix B.1 – VBA code for the multi-objective simulation

```
Sub Flowchart24()
    Dim ws As Worksheet
    Set ws = ThisWorkbook.Sheets("Simulation_2023_Hourly")

    Dim lastRow As Long
    lastRow = ws.Cells(ws.Rows.Count, "A").End(xlUp).Row

    Dim max_vol As Double, max_vol_sec As Double, min_vol_sec As Double,
wchp_max As Double
    max_vol = 1250 'm^3
    max_vol_sec = 0.75 '%
    min_vol_sec = 0.25 '%
    wchp_max = 550  'kwh

    Dim f As Double
    f = 2 'kwh/m^3, conversion factor of biogas

    Dim i As Long
    For i = 3 To lastRow
        ' Input variables
        Dim hr As Double, wpv As Double, wload As Double, vol As Double, qb
As Double, wchp As Double, wb As Double
        Dim e_buy As String, e_sell As Double

        hr = ws.Cells(i, 1).Value
        e_buy = ws.Cells(i, 2).Value
        e_sell = ws.Cells(i, 3).Value
        wpv = ws.Cells(i, 4).Value
        wload = ws.Cells(i, 5).Value
        vol = ws.Cells(i, 6).Value
        qb = ws.Cells(i, 7).Value

        If i = 3 Then
            wchp = 0
        Else
            wchp = ws.Cells(i - 1, 9).Value
        End If

        wb = f * qb
        ws.Cells(i, 8).Value = wb
```

```
        ' Energy accounting variables
        Dim energy_in As Double, energy_out As Double, energy_stored As
Double, leftover_energy As Double

        ' Initial energy input
        energy_in = wpv + wb + (vol * f)

        ' Decision variables
        Dim d1 As Boolean, d2 As Boolean, d3 As Boolean, d4 As Boolean, d5
As Boolean
        d1 = (wb >= wload)
        d2 = (wpv >= wload)
        d3 = (wpv + wb >= wload)
        d4 = (e_buy = "Mid-Peak_W" Or e_buy = "Peak_W" Or e_buy = "Off-
Peak_W" Or e_buy = "Mid-Peak_S" Or e_buy = "Peak_S" Or e_buy = "Off-
Peak_S")
        d5 = (vol >= max_vol * min_vol_sec) And d4

        ' Initialize output variables
        Dim new_vol As Double, wchp_out As Double, qchp_out As Double,
wbl_out As Double, wpvl_out As Double
        Dim wl_out As Double, wsell_out As Double, wbuy_out As Double,
qtorch As Double, qchp2_out As Double, wchp2_out As Double

        ' Decision tree
        If d1 Then
            ' Handle case where biogas can meet load
            wchp_out = Application.Min(wchp_max, wload)
            wbl_out = wload
            wpvl_out = 0
            wl_out = wload
            wsell_out = wpv + (wchp_out - wload)
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d2 Then
            ' Handle case where PV can meet load
            wchp_out = Application.Min(wchp_max, wb)
            wbl_out = 0
            wpvl_out = wload
            wl_out = wload
            wsell_out = (wchp_out + (wpv - wload))
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d3 Then
            ' Handle case where PV + biogas can meet load
            wchp_out = wload - wpv
            wbl_out = wchp_out
            wpvl_out = wpv
            wl_out = wload
            wsell_out = 0
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d5 Then
            ' Use stored volume when price is high and volume is higher
than 25%
            Dim available_energy As Double
            available_energy = vol * f
            If available_energy >= (wload - wpv - wb) Then
                ' Stored energy can cover the deficit
                wchp_out = Application.Min(wchp_max, wload - wpv)
```

```
                wbl_out = wload - wpv
                wpvl_out = wpv
                wl_out = wload
                wsell_out = 0
                wbuy_out = 0
                leftover_energy = wb - (wchp_out - (wload - wpv - wb))
                new_vol = vol - ((wload - wpv - wb) / f)
            Else
                ' Stored energy can't cover all the deficit, use what we
can
                wchp_out = Application.Min(wchp_max, wb + available_energy)
                wbl_out = wb + available_energy
                wpvl_out = wpv
                wl_out = wload
                wsell_out = 0
                wbuy_out = wload - wpv - wbl_out
                leftover_energy = 0
                new_vol = 0 ' We've used all stored energy
            End If
        Else
            ' Handle case where external power is needed
            wchp_out = Application.Min(wchp_max, wb)
            wbl_out = wchp_out
            wpvl_out = wpv
            wl_out = wload
            wsell_out = 0
            wbuy_out = wload - wpv - wchp_out
            leftover_energy = wb - wchp_out
        End If

        ' Handle leftover energy
        If leftover_energy > 0 Then
            If Not IsEmpty(new_vol) Then
                new_vol = Application.Min(max_vol, new_vol +
(leftover_energy / f))
            Else
                new_vol = Application.Min(max_vol, vol + (leftover_energy /
f))
            End If
            qtorch = Application.Max(0, (leftover_energy / f) - (max_vol -
vol))
            qchp2_out = qtorch
            wchp2_out = qchp2_out * f
        ElseIf IsEmpty(new_vol) Then
            new_vol = vol
            qtorch = 0
            qchp2_out = 0
            wchp2_out = 0
        End If

        ' Calculate energy output and stored
        energy_out = wl_out + wsell_out + wchp2_out
        energy_stored = (new_vol - vol) * f

        ' Check energy balance
        Dim energy_diff As Double
        energy_diff = Abs((energy_in + wbuy_out) - (energy_out +
energy_stored))
```

```
        ' Log if energy difference is significant
        If energy_diff > 0.001 Then ' Tolerance of 0.001 kWh
            Debug.Print "Energy imbalance at hour " & hr & ": " &
energy_diff & " kWh"
            Debug.Print "In: " & energy_in & ", Out: " & energy_out & ",
Stored: " & energy_stored & ", Bought: " & wbuy_out
        End If

        ' Update worksheet
        ws.Cells(i, 9).Value = wchp_out
        ws.Cells(i, 10).Value = wchp_out / f
        ws.Cells(i, 11).Value = wbl_out
        ws.Cells(i, 12).Value = wpvl_out
        ws.Cells(i, 13).Value = wl_out
        ws.Cells(i, 14).Value = wsell_out
        ws.Cells(i, 15).Value = wbuy_out
        ws.Cells(i, 16).Value = qtorch
        ws.Cells(i, 17).Value = qchp2_out
        ws.Cells(i, 18).Value = wchp2_out
        ws.Cells(i, 19).Value = new_vol
    Next i
End Sub
```

Appendix B.2 – VBA code for the multi-objective simulation, with PV and biogas as sources of energy and preference for using stored biogas

```
Sub Flowchart24()
    Dim ws As Worksheet
    Set ws = ThisWorkbook.Sheets("Simulation_2023_Hourly_PV_2")

    Dim lastRow As Long
    lastRow = ws.Cells(ws.Rows.Count, "A").End(xlUp).Row

    Dim max_vol As Double, high_vol_threshold As Double, mid_vol_threshold
As Double, low_vol_threshold As Double, wchp_max As Double
    max_vol = 1250 'm^3
    high_vol_threshold = 0.75 '% of max_vol
    mid_vol_threshold = 0.4  '% of max_vol
    low_vol_threshold = 0.15 '% of max_vol
    wchp_max = 550  'kwh

    Dim f As Double
    f = 2 'kwh/m^3, conversion factor of biogas

    Dim i As Long
    For i = 3 To lastRow
        ' Input variables
        Dim hr As Double, wpv As Double, wload As Double, vol As Double, qb
As Double, wb As Double
        Dim e_buy As String, e_sell As Double

        hr = ws.Cells(i, 1).Value
        e_buy = ws.Cells(i, 2).Value
        e_sell = ws.Cells(i, 3).Value
        wpv = ws.Cells(i, 4).Value
```

```
        wload = ws.Cells(i, 5).Value
        vol = ws.Cells(i, 6).Value
        qb = ws.Cells(i, 7).Value

        wb = f * qb
        ws.Cells(i, 8).Value = wb

        ' Energy accounting variables
        Dim energy_in As Double, energy_out As Double, energy_stored As
Double

        ' Initial energy input
        energy_in = wpv + wb + (vol * f)

        ' Initialize output variables
        Dim new_vol As Double, wchp_out As Double, wbl_out As Double,
wpvl_out As Double
        Dim wl_out As Double, wsell_out As Double, wbuy_out As Double,
qtorch As Double

        ' Decision tree
        If wb >= wload Then
            ' Biogas can meet load
            wchp_out = wload
            wbl_out = wload
            wpvl_out = 0
            wl_out = wload
            wbuy_out = 0

            ' Store excess biogas if possible, otherwise use for CHP
            If vol < max_vol Then
                new_vol = Application.Min(max_vol, vol + (wb - wload) / f)
                wsell_out = wpv
            Else
                new_vol = max_vol
                wchp_out = Application.Min(wchp_max, wb)
                wsell_out = wpv + (wchp_out - wload)
            End If
        ElseIf vol >= max_vol * mid_vol_threshold And (wb + vol * f) >=
wload Then
            ' Biogas + reserves can meet load (when reserves > 40%)
            wchp_out = wload
            wbl_out = wload
            wpvl_out = 0
            wl_out = wload
            wbuy_out = 0
            new_vol = vol - (wload - wb) / f
            wsell_out = wpv
        ElseIf wpv >= wload Then
            ' PV can meet load
            wchp_out = 0
            wbl_out = 0
            wpvl_out = wload
            wl_out = wload
            wbuy_out = 0
            new_vol = Application.Min(max_vol, vol + wb / f)
            wsell_out = wpv - wload
        ElseIf wpv + wb >= wload Then
            ' PV + biogas can meet load
```

```
            wchp_out = wload - wpv
            wbl_out = wchp_out
            wpvl_out = wpv
            wl_out = wload
            wbuy_out = 0
            new_vol = Application.Min(max_vol, vol + (wb - wchp_out) / f)
            wsell_out = 0
        ElseIf vol >= max_vol * high_vol_threshold Then
            ' Reserves are high, use stored energy
            Dim available_energy As Double
            available_energy = vol * f
            If available_energy >= (wload - wpv - wb) Then
                ' Stored energy can cover the deficit
                wchp_out = wload - wpv
                wbl_out = wload - wpv
                wpvl_out = wpv
                wl_out = wload
                wbuy_out = 0
                new_vol = vol - (wload - wpv - wb) / f
                wsell_out = 0
            Else
                ' Stored energy can't cover all the deficit, use what we
can
                wchp_out = wb + available_energy
                wbl_out = wb + available_energy
                wpvl_out = wpv
                wl_out = wload
                wbuy_out = wload - wpv - wbl_out
                new_vol = 0 ' We've used all stored energy
                wsell_out = 0
            End If
        Else
            ' External power is needed
            wchp_out = wb
            wbl_out = wb
            wpvl_out = wpv
            wl_out = wload
            wbuy_out = wload - wpv - wb
            new_vol = Application.Min(max_vol, vol + wb / f)
            wsell_out = 0
        End If

        ' Handle excess energy (if any)
        Dim excess_energy As Double
        excess_energy = energy_in - (wl_out + wsell_out + (new_vol - vol) *
f)

        If excess_energy > 0 Then
            If vol < max_vol * high_vol_threshold Then
                ' Prioritize storing energy if volume is below high
threshold
                new_vol = Application.Min(max_vol, new_vol + excess_energy
/ f)
                qtorch = 0
            Else
                ' Use qtorch for remaining energy
                qtorch = excess_energy / f
                wsell_out = wsell_out + excess_energy
            End If
        Else
```

```
            qtorch = 0
        End If

        ' Calculate energy output and stored
        energy_out = wl_out + wsell_out
        energy_stored = (new_vol - vol) * f

        ' Check energy balance
        Dim energy_diff As Double
        energy_diff = Abs((energy_in + wbuy_out) - (energy_out +
energy_stored))

        ' Log if energy difference is significant
        If energy_diff > 0.001 Then ' Tolerance of 0.001 kWh
            Debug.Print "Energy imbalance at hour " & hr & ": " &
energy_diff & " kWh"
            Debug.Print "In: " & energy_in & ", Out: " & energy_out & ",
Stored: " & energy_stored & ", Bought: " & wbuy_out
        End If

        ' Update worksheet
        ws.Cells(i, 9).Value = wchp_out
        ws.Cells(i, 10).Value = wchp_out / f
        ws.Cells(i, 11).Value = wbl_out
        ws.Cells(i, 12).Value = wpvl_out
        ws.Cells(i, 13).Value = wl_out
        ws.Cells(i, 14).Value = wsell_out
        ws.Cells(i, 15).Value = wbuy_out
        ws.Cells(i, 16).Value = qtorch
        ws.Cells(i, 17).Value = 0 ' qchp2_out is no longer used
        ws.Cells(i, 18).Value = 0 ' wchp2_out is no longer used
        ws.Cells(i, 19).Value = new_vol
    Next i
End Sub
```

Appendix B.3 – VBA code for the energy purchase minimization objective simulation

```
Sub Flowchart24()
    Dim ws As Worksheet
    Set ws = ThisWorkbook.Sheets("Simulation_2023_Hourly_PV")

    Dim lastRow As Long
    lastRow = ws.Cells(ws.Rows.Count, "A").End(xlUp).Row

    Dim max_vol As Double, max_vol_sec As Double, min_vol_sec As Double,
wchp_max As Double, mid_vol_sec As Double
    max_vol = 1250 'm^3
    max_vol_sec = 0.75 '%
    min_vol_sec = 0.25 '%
    mid_vol_sec = 0.4  '%
    wchp_max = 550  'kwh

    Dim f As Double
    f = 2 'kwh/m^3, conversion factor of biogas
```

```
    Dim i As Long
    For i = 3 To lastRow
        ' Input variables
        Dim hr As Double, wpv As Double, wload As Double, vol As Double, qb
As Double, wchp As Double, wb As Double
        Dim e_buy As String, e_sell As Double

        hr = ws.Cells(i, 1).Value
        e_buy = ws.Cells(i, 2).Value
        e_sell = ws.Cells(i, 3).Value
        wpv = ws.Cells(i, 4).Value
        wload = ws.Cells(i, 5).Value
        vol = ws.Cells(i, 6).Value
        qb = ws.Cells(i, 7).Value

        If i = 3 Then
            wchp = 0
        Else
            wchp = ws.Cells(i - 1, 9).Value
        End If

        wb = f * qb
        ws.Cells(i, 8).Value = wb

        ' Energy accounting variables
        Dim energy_in As Double, energy_out As Double, energy_stored As
Double, leftover_energy As Double

        ' Initial energy input
        energy_in = wpv + wb + (vol * f)

        ' Decision variables
        Dim d1 As Boolean, d2 As Boolean, d3 As Boolean, d4 As Boolean, d5
As Boolean, d6 As Boolean
        d1 = (wb >= wload)
        d2 = (wpv >= wload)
        d3 = (wpv + wb >= wload)
        d4 = (e_buy = "Mid-Peak_W" Or e_buy = "Peak_W" Or e_buy = "Off-
Peak_W" Or "Mid-Peak_S" Or e_buy = "Peak_S" Or e_buy = "Off-Peak_S")
        d5 = (vol >= max_vol * min_vol_sec) And d9
        d6 = (vol > max_vol * mid_vol_sec)

        ' Initialize output variables
        Dim new_vol As Double, wchp_out As Double, qchp_out As Double,
wbl_out As Double, wpvl_out As Double
        Dim wl_out As Double, wsell_out As Double, wbuy_out As Double,
qtorch As Double, qchp2_out As Double, wchp2_out As Double

        ' Decision tree
        If d1 Then
            ' Handle case where biogas can meet load
            wchp_out = Application.Min(wchp_max, wload)
            wbl_out = wload
            wpvl_out = 0
            wl_out = wload
            wsell_out = wpv + (wchp_out - wload)
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d2 Then
```

```
            ' Handle case where PV can meet load
            wchp_out = Application.Min(wchp_max, wb)
            wbl_out = 0
            wpvl_out = wload
            wl_out = wload
            wsell_out = (wchp_out + (wpv - wload))
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d3 Then
            ' Handle case where PV + biogas can meet load
            wchp_out = wload - wpv
            wbl_out = wchp_out
            wpvl_out = wpv
            wl_out = wload
            wsell_out = 0
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d5 Or d6 Then
            ' Use stored volume when price is high and volume is higher
than 25%, or when volume > 40%
            Dim available_energy As Double
            available_energy = vol * f
            If available_energy >= (wload - wpv - wb) Then
                ' Stored energy can cover the deficit
                wchp_out = Application.Min(wchp_max, wload - wpv)
                wbl_out = wload - wpv
                wpvl_out = wpv
                wl_out = wload
                wsell_out = 0
                wbuy_out = 0
                leftover_energy = wb - (wchp_out - (wload - wpv - wb))
                new_vol = vol - ((wload - wpv - wb) / f)
            Else
                ' Stored energy can't cover all the deficit, use what we
can
                wchp_out = Application.Min(wchp_max, wb + available_energy)
                wbl_out = wchp_out
                wpvl_out = wpv
                wl_out = wload
                wsell_out = 0
                wbuy_out = wload - wpv - wbl_out
                leftover_energy = 0
                new_vol = 0 ' We've used all stored energy
            End If
        Else
            ' Handle case where external power is needed
            wchp_out = Application.Min(wchp_max, wb)
            wbl_out = wchp_out
            wpvl_out = wpv
            wl_out = wload
            wsell_out = 0
            wbuy_out = wload - wpv - wchp_out
            leftover_energy = wb - wchp_out
        End If

        ' Handle leftover energy
        If leftover_energy > 0 Then
            If Not IsEmpty(new_vol) Then
```

```
                new_vol = Application.Min(max_vol, new_vol +
(leftover_energy / f))
            Else
                new_vol = Application.Min(max_vol, vol + (leftover_energy /
f))
            End If
            qtorch = Application.Max(0, (leftover_energy / f) - (max_vol -
vol))
            qchp2_out = qtorch
            wchp2_out = qchp2_out * f
        ElseIf IsEmpty(new_vol) Then
            new_vol = vol
            qtorch = 0
            qchp2_out = 0
            wchp2_out = 0
        End If

        ' Calculate energy output and stored
        energy_out = wl_out + wsell_out + wchp2_out
        energy_stored = (new_vol - vol) * f

        ' Check energy balance
        Dim energy_diff As Double
        energy_diff = Abs((energy_in + wbuy_out) - (energy_out +
energy_stored))

        ' Log if energy difference is significant
        If energy_diff > 0.001 Then ' Tolerance of 0.001 kWh
            Debug.Print "Energy imbalance at hour " & hr & ": " &
energy_diff & " kWh"
            Debug.Print "In: " & energy_in & ", Out: " & energy_out & ",
Stored: " & energy_stored & ", Bought: " & wbuy_out
        End If

        ' Update worksheet
        ws.Cells(i, 9).Value = wchp_out
        ws.Cells(i, 10).Value = wchp_out / f
        ws.Cells(i, 11).Value = wbl_out
        ws.Cells(i, 12).Value = wpvl_out
        ws.Cells(i, 13).Value = wl_out
        ws.Cells(i, 14).Value = wsell_out
        ws.Cells(i, 15).Value = wbuy_out
        ws.Cells(i, 16).Value = qtorch
        ws.Cells(i, 17).Value = qchp2_out
        ws.Cells(i, 18).Value = wchp2_out
        ws.Cells(i, 19).Value = new_vol
    Next i
End Sub
```

Appendix B.4 – VBA code for the burnt biogas minimization objective simulation

```
Sub Flowchart24()
    Dim ws As Worksheet
    Set ws = ThisWorkbook.Sheets("Simulation_2023_Hourly_PV_Torch")

    Dim lastRow As Long
```

```
    lastRow = ws.Cells(ws.Rows.Count, "A").End(xlUp).Row

    Dim max_vol As Double, max_vol_sec As Double, min_vol_sec As Double,
wchp_max As Double
    max_vol = 1250 ' m^3
    max_vol_sec = 0.9 ' %
    min_vol_sec = 0.1 ' %
    wchp_max = 550  ' kwh

    Dim f As Double
    f = 2 'kwh/m^3, conversion factor of biogas

    Dim i As Long
    For i = 3 To lastRow
        ' Input variables
        Dim hr As Double, wpv As Double, wload As Double, vol As Double, qb
As Double, wchp As Double, wb As Double
        Dim e_buy As String, e_sell As Double

        hr = ws.Cells(i, 1).Value
        e_buy = ws.Cells(i, 2).Value
        e_sell = ws.Cells(i, 3).Value
        wpv = ws.Cells(i, 4).Value
        wload = ws.Cells(i, 5).Value
        vol = ws.Cells(i, 6).Value
        qb = ws.Cells(i, 7).Value

        If i = 3 Then
            wchp = 0
        Else
            wchp = ws.Cells(i - 1, 9).Value
        End If

        wb = f * qb
        ws.Cells(i, 8).Value = wb

        ' Energy accounting variables
        Dim energy_in As Double, energy_out As Double, energy_stored As
Double, leftover_energy As Double

        ' Initial energy input
        energy_in = wpv + wb + (vol * f)

        ' Decision variables
        Dim d1 As Boolean, d2 As Boolean, d3 As Boolean, d4 As Boolean, d5
As Boolean, d6 As Boolean, d7 As Boolean

        d1 = (wb >= wload)
        d2 = (vol >= max_vol * min_vol_sec)
        d3 = (wpv >= wload)
        d4 = (wpv + wb >= wload)
        d5 = (wb >= wchp_max)
        d6 = (e_buy = "Mid-Peak_W" Or e_buy = "Peak_W" Or "Mid-Peak_S" Or
e_buy = "Peak_S")
        d7 = d2 And d6 ' Use stored volume when price is high and volume is
above minimum threshold

        ' Initialize output variables
```

```
        Dim new_vol As Double, wchp_out As Double, qchp_out As Double,
wbl_out As Double, wpvl_out As Double
        Dim wl_out As Double, wsell_out As Double, wbuy_out As Double,
wtorch As Double

        If d5 Then
            ' Prioritize using biogas when abundant, run CHP at maximum
            wchp_out = wchp_max
            wbl_out = wchp_out
            wpvl_out = Application.Min(wpv, wload - wchp_out)
            wl_out = wload
            wsell_out = Application.Max(0, wpv - wpvl_out)
            wbuy_out = Application.Max(0, wload - wchp_out - wpvl_out)
            leftover_energy = wb - wchp_out
        ElseIf d1 Then
            ' Use biogas to meet load, run CHP up to maximum
            wchp_out = Application.Min(wchp_max, wload)
            wbl_out = wload
            wpvl_out = 0
            wl_out = wload
            wsell_out = wpv + (wb - wchp_out)
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d3 Then
            ' Use PV when sufficient, run CHP with remaining biogas
            wchp_out = Application.Min(wchp_max, wb)
            wbl_out = wchp_out
            wpvl_out = wload
            wl_out = wload
            wsell_out = (wpv - wload) + wchp_out
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d4 Then
            ' Use combination of PV and biogas
            wchp_out = Application.Min(wchp_max, wload - wpv)
            wbl_out = wchp_out
            wpvl_out = wpv
            wl_out = wload
            wsell_out = 0
            wbuy_out = 0
            leftover_energy = wb - wchp_out
        ElseIf d7 Then
            ' Use stored volume when price is high and volume is sufficient
            Dim available_energy As Double
            available_energy = Application.Min((vol - max_vol *
min_vol_sec) * f, wchp_max)
            wchp_out = Application.Min(available_energy, wload - wpv)
            wbl_out = wchp_out
            wpvl_out = wpv
            wl_out = wload
            wsell_out = 0
            wbuy_out = Application.Max(0, wload - wpv - wchp_out)
            leftover_energy = wb
            new_vol = vol - (wchp_out / f)
        Else
            ' Default case: use available biogas and buy remaining
            wchp_out = Application.Min(wchp_max, wb)
            wbl_out = wchp_out
            wpvl_out = wpv
            wl_out = wload
```

```
            wsell_out = 0
            wbuy_out = Application.Max(0, wload - wpv - wchp_out)
            leftover_energy = wb - wchp_out
        End If

        ' Handle leftover energy and calculate q_torch
        If leftover_energy > 0 Then
            ' Calculate how much energy can be stored
            Dim storable_energy As Double
            storable_energy = (max_vol - vol) * f

            If leftover_energy <= storable_energy Then
                ' All leftover energy can be stored
                new_vol = vol + (leftover_energy / f)
                wtorch = 0
            Else
                ' Some energy might need to be burned
                new_vol = max_vol
                If wchp_out = wchp_max Then
                    ' Only redirect to q_torch if CHP is at maximum
capacity
                    wtorch = leftover_energy - storable_energy
                Else
                    ' Increase CHP output if possible, otherwise energy is
lost
                    Dim additional_chp As Double
                    additional_chp = Application.Min(wchp_max - wchp_out,
leftover_energy - storable_energy)
                    wchp_out = wchp_out + additional_chp
                    wbl_out = wbl_out + additional_chp
                    wsell_out = wsell_out + additional_chp
                    wtorch = leftover_energy - storable_energy -
additional_chp
                End If
            End If
        Else
            If IsEmpty(new_vol) Then
                new_vol = vol
            End If
            wtorch = 0
        End If

        ' Calculate energy output and stored
        energy_out = wl_out + wsell_out + wtorch
        energy_stored = (new_vol - vol) * f

        ' Check energy balance
        Dim energy_diff As Double
        energy_diff = Abs((energy_in + wbuy_out) - (energy_out +
energy_stored))

        ' Log if energy difference is significant
        If energy_diff > 0.001 Then ' Tolerance of 0.001 kWh
            Debug.Print "Energy imbalance at hour " & hr & ": " &
energy_diff & " kWh"
            Debug.Print "In: " & energy_in & ", Out: " & energy_out & ",
Stored: " & energy_stored & ", Bought: " & wbuy_out & ", Torched: " &
wtorch
        End If
```

```
        ' Update worksheet
        ws.Cells(i, 9).Value = wchp_out
        ws.Cells(i, 10).Value = wchp_out / f
        ws.Cells(i, 11).Value = wbl_out
        ws.Cells(i, 12).Value = wpvl_out
        ws.Cells(i, 13).Value = wl_out
        ws.Cells(i, 14).Value = wsell_out
        ws.Cells(i, 15).Value = wbuy_out
        ws.Cells(i, 16).Value = wtorch / f
        ws.Cells(i, 17).Value = wtorch / f
        ws.Cells(i, 18).Value = wtorch
        ws.Cells(i, 19).Value = new_vol
    Next i
End Sub
```

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DECLARAÇÃO DE INTEGRIDADE

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ISEP, Porto, 1 de outubro de 2024

Rúben Ramalho Gonçalves