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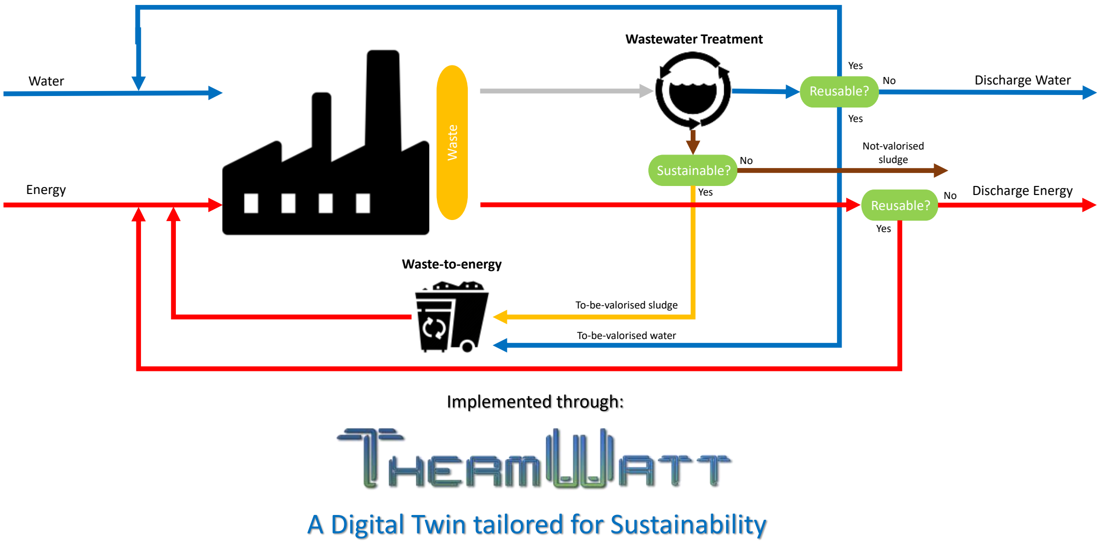

Simulation and Optimisation of Water and Energy Integration Systems (WEIS)

An Innovative Approach for Process Industries

Delfim Miguel Marmelo Castro Oliveira

Supervisor: Doctor Henrique Aníbal Santos de Matos

Co-Supervisor: Doctor Muriel de Carvalho Iten

Thesis approved in public session to obtain the PhD Degree in

Sustainable Energy Systems

Jury final classification: **Pass with Distinction**

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Funding Institution

ISQ – Instituto de Soldadura e Qualidade

2023

The measure of a man is what he does with power.

Plato, 428/427–348/347 B.C.E.

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Acknowledgements

First of all, I would like to thank my parents, most specially my mother, whose unconditional love had shaped me to the man I am today. I would also want to thank my sister Engineer Rita Castro Oliveira who was since the beginning my greatest friend, and who is also set to deliver her Master thesis on Computer Science and Engineering in this year of 2023.

During the almost 4-year span of my PhD, so many people had left their mark on me. Shall exist a shadow of doubt, it is to note that these acknowledgements are dedicated to the ones that had an actual positive contribution without proceeding with harsh and unnecessary criticism (a note that I had also performed in my Master thesis back in 2018).

I would like to acknowledge a group of people that are representants within each one of the entities I belong to and in which my PhD work has been based. On the side of Instituto Superior Técnico and CERENA – Centro de Recursos Naturais e Ambiente, I would like to give the biggest and much appreciated thank to my doctoral advisor Prof. Henrique Matos, who has been accompanying the academic side of my Researcher since the beginning of it and giving me the most precious and wise advice. On the side of ISQ – Instituto de Soldadura e Qualidade (the enterprise in which I am a collaborator since 2018, 6 years the date of the ending of this PhD work), I would like to thank Ricardo Rato, Director of the R&Di division in which I am a Researcher, and João Safara, Member of ISQ Board of Administrators, who have been supporting my projects and initiatives. I would also like to thank Prof. Paulo Ferrão, coordinator of the Sustainable Energy Systems program, who had been a great influence on my growing will to exploit all the areas related to sustainable systems.

To my colleagues on the ISQ R&Di division, at Low Carbon & Resource Efficiency, Intelligent and Digital Systems, Materials & Technologies, Training & Qualifications, Programme Management and Contract Management, I would like to thank all the support in the last years. It would be unfair to identify people in particular, the ones that know my appreciation and that give me appreciation in return will recognize my acknowledgement. To my colleagues on CERENA, a big thank you, in particular to my colleagues on LabSOP and the Energy Group.

A special appreciation to my grandfather and grandmother, who despite not being physically present are always alive in my memory.

To all my close friends who have a wise word of support and who were always there in the most difficult times.

I would like to finish by citing a phrase that I had wrote at hand in the memory book existing in the surroundings of the Panathenaic Stadium in Athens: *Power is the combination of potential and wisdom to use it*. I hope you all understand my message!

Miguel Castro Oliveira

July 2023, revised January 2024

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Abstract

The improvement of water and energy use is an important concern to diminish economic issues and the total environmental burden produced by the activities of end-us sectors. Industry is one of the main contributors of the final energy consumption, associated GHG emissions, freshwater consumption and wastewater discharges. The concept of water-energy nexus has been introduced to analyse the interdependencies between water and energy use. In its turn, the methodology of process integration has been introduced to exploit the benefits of the interdependencies between several resources. In this work, two innovative assets are introduced: the concept of Water and Energy Integration Systems (WEIS) and a computation tool created for the purpose to assist on Engineering projects related to the installation of these systems designated as ThermWatt (developed with the Modelica and Python languages). Two case-studies are analysed and assessed. For respectively case-studies 1 and 2, it was assessed an 8.80% and 7.92% total energy consumption reduction, a 23.71% and 38.57% total water consumption reduction in the studied water system have been estimated. It has been assessed a payback time of 22 months for case-study 1 and 34 months for case-study 2. It has also been assessed a 2.42 and 1.76 kton $\mathrm{CO}_{2,\mathrm{eq}}$/year for case-studies 1 and 2, respectively. The results for final assessment indicators proved that the conceptualized WEIS projects are robust in terms of eco-efficiency, circular economy potential and strategic objective achievement potential, with a 6.46% and 4.00% improvement for the aggregated eco-efficiency indicator having been obtained for respectively case-studies 1 and 2, a null water discharge for both case-studies and a level of 8.58% and 6.69% of recirculated heat over total energy consumption.

Keywords

Water and Energy Integration Systems, water-energy nexus, energy recovery, water recirculation, ThermWatt tool

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Resumo

A melhoria do uso de água e energia é uma preocupação importante para diminuir os problemas económicos e a carga ambiental total produzida pelas atividades dos setores de uso final. A indústria é um dos principais contribuintes do consumo final de energia e das emissões associadas de GEE, consumos de água doce e descargas de águas residuais. O conceito de nexus água-energia foi introduzido para analisar as interdependências entre o uso de água e energia. Por sua vez, a metodologia de integração de processos foi introduzida para explorar os benefícios das interdependências entre diversos recursos. Neste trabalho, são apresentados dois ativos inovadores: o conceito de Sistemas de Integração de Água e Energia (SIAE) e uma ferramenta computacional criada com a finalidade de ser usada em projetos de Engenharia relacionados com a instalação destes sistemas denominada de ThermWatt (desenvolvida com as linguages Modelica e Python). Dois casos-estudo são analisados e avaliados. Para os casos-estudo 1 e 2, foram respetivamente estimadas reduções de 8,80% e 7,92% no consumo total de energia, estimando-se uma redução no consumo total de água de 23,71% e 38,57% no sistema de água estudado. Foi avaliado um tempo de retorno de 22 meses para o caso-estudo 1 e 34 meses para o caso-estudo 2. Também foi avaliado um 1,82 e 1,76 kton $\mathrm{CO_{2,eq}}$/ano para os casos-estudo 1 e 2, respetivamente. Os resultados para os indicadores da avaliação final comprovaram que os projetos de SIAE conceptualizados são robustos em termos de ecoeficiência, potencial de economia circular e potencial de alcance de objetivos estratégicos, com uma melhoria de 6,67% e 4,00% para o indicador agregado de ecoeficiência obtido para os casos-estudo 1 e 2, respetivamente, uma descarga de água nula para ambos os casos-estudo e um nível de 8,58% e 6,69% de calor reciclado sobre o consumo total de energia.

Palavras-chave

Sistemas de Integração de Água e Energia, nexus água-energia, recuperação de energia, recirculação de água, ThermWatt tool

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Publications and Events

In the scope of this thesis, several publications have been generated, which contribute and receive contribution from and to the contents elaborated for the thesis, with these being listed in Table i1. A distinction is performed between main publications (direct contributions from or to the contents of the thesis) and secondary publications (developed from in the scope of the same project and initiatives that are associated to the thesis but not being a direct contribution from or to). Furthermore, the whole developed work also made possible the participation of the author within several events, which are listed in Table i2.

Table i1. List of developed publications

Typology	Title	Year
Main Publications		
Literature Review	Castro Oliveira M, Iten M, Cruz, P.L, Monteiro H.M. Review on Energy Efficiency Progresses, Technologies and Strategies in the Ceramic Sector Focusing on Waste Heat Recovery. Energies. **https://doi.org/10.3390/en13226096**	2020
	Castro Oliveira M, Iten M, Matos H.A. Review of Thermochemical Technologies for Water and Energy Integration Systems: Energy Storage and Recovery. Sustainability. **https://doi.org/10.3390/su14127506**	2022
	Castro Oliveira M, Iten M, Matos H.A. Review on Water and Energy Integration in Process Industry: Water-Heat Nexus. Sustainability. **https://doi.org/10.3390/su14137954**	2022
Research (Simulation and Optimisation Models)	Castro Oliveira M, Iten M, Matos H.A. Assessment of energy efficiency improvement in ceramic industry through waste heat recovery modelling. ESCAPE31 (31st European Symposium on Computer-Aided Process Engineering). **https://doi.org/10.1016/B978-0-323-88506-5.50256-4**	2021
	Castro Oliveira M, Vieira S.M, Iten M, Matos H.A. Optimization of Water-Energy Networks (WEN) in Process Industry: Implementation of non-linear and multi-objective models. Frontiers in Chemical Engineering. **https://doi.org/10.3389/fceng.2021.750411**	2022
	Castro Oliveira M, Coelho P.J, Iten M, Matos H.A. Modelling of Heat-Driven Water Treatment Systems: Multi-Effect Distillation (MED) model in Modelica. ESCAPE32 (32nd European Symposium on Computer-Aided Process Engineering). **https://doi.org/10.1016/B978-0-323-95879-0.50067-9**	2022
	Castro Oliveira M, Iten M, Matos H.A. Simulation and assessment of an integrated thermal processes and Organic Rankine Cycle (ORC) system with Modelica. Energy Reports. **https://doi.org/10.1016/j.egyr.2022.10.268**	2022
	Castro Oliveira M, Iten M, Matos H.A. Simultaneous optimisation of energy recovery and water recirculation in a ceramic plant. ESCAPE33 (33rd European Symposium on Computer-Aided Process Engineering). **https://doi.org/10.1016/B978-0-443-15274-0.50443-1**	2023
	Castro Oliveira M, Castro Oliveira R, Matos H.A. Dynamic simulation and optimisation of water and energy consumption in a ceramic plant: Application of the customised ThermWatt computational tool. ESCAPE34–PSE24 (34th European Symposium on Computer-Aided Process Engineering). **https://shorturl.at/lsHVW**	2024
Research	Iten M, Fernandes U, Castro Oliveira M. Framework to Assess Eco-Efficiency	2021

(Post-processing Assessment)	Improvement: Case Study of a Meat Production Industry. Energy Reports. **https://doi.org/10.1016/j.egyr.2021.09.120**	
	Castro Oliveira M, Matos H.A. Assessment of Sustainability and Strategic aims for Water and Energy Integration Systems: Case-studies of the Process Industry in Portugal. **https://doi.org/10.3390/en17010195**	2023
Newspaper Articles	Castro Oliveira M. Sustentabilidade, nexus água-energia e escassez de recursos. **https://www.publico.pt/2023/11/28/ciencia/noticia/sustentabilidade-nexus-aguaenergia-escassez-recursos-2071500**	2023
	Secondary Publications	
Research (Simulation and Optimisation Models)	Castro Oliveira M, Iten M. Modelling of a solar thermal energy system for energy efficiency improvement in a ceramic plant. Renewable Energy and Environmental Sustainability. **https://doi.org/10.1051/rees/2021029**	2021
	Castro Oliveira M, Iten M, Fernandes U. Modelling of a solar thermal energy system for energy efficiency improvement in a ceramic plant. World Renewable Energy Congress (WREC). **https://doi.org/10.1007/978-3-030-76221-6_91**	2022
	Castro Oliveira M, Iten M, Matos H.A. An open-source tool for water, energy and waste management integrated assessment. **https://doi.org/10.5281/zenodo.7706656**	2023
	Castro Oliveira M, Iten M, Matos H.A. Closing the loop through water and heat valorisation in industrial processes – A circular economy approach. **https://doi.org/10.5281/zenodo.7706665**	2023

Table i2. List of event participations

Event	Title of Work(s)	Year
	Conferences	
ESCAPE31	Castro Oliveira M, Iten M, Matos H.A. Assessment of energy efficiency improvement in ceramic industry through waste heat recovery modelling. Escape-31 (31st European Symposium on Computer-Aided Process Engineering). **https://sustainable-future.webnode.pt/posterescape31**	2021
WREC2020	Castro Oliveira M, Iten M, Fernandes U. Modelling of a solar thermal energy system for energy efficiency improvement in a ceramic plant. World Renewable Energy Congress (WREC). **https://doi.org/10.1007/978-3-030-76221-6_91**	2021
ESCAPE32	Castro Oliveira M, Coelho P.J, Iten M, Matos H.A. Modelling of Heat-Driven Water Treatment Systems: Multi-Effect Distillation (MED) model in Modelica. Escape-32 (32nd European Symposium on Computer-Aided Process Engineering). **https://sustainable-future.webnode.pt/poster-escape32**	2022
WWEM 2022	Castro Oliveira M, Iten M, Matos H.A. An open-source tool for water, energy and waste management integrated assessment. **https://doi.org/10.5281/zenodo.7706656**	2022
	Iten M, Castro Oliveira M, Matos H.A. Closing the loop through water and heat valorisation in industrial processes – A circular economy approach. **https://doi.org/10.5281/zenodo.7706665**	
REEE 2022	Castro Oliveira M, Iten M, Matos H.A. Simulation and assessment of an integrated thermal processes and Organic Rankine Cycle (ORC) system with Modelica. Energy Reports. **https://doi.org/10.1016/j.egyr.2022.10.268**	2022
ESCAPE33	Castro Oliveira M, Matos H.A. Simultaneous optimisation of energy recovery and water recirculation in a ceramic plant. **https://sustainable-future.webnode.pt/poster-escape33**	2023

Fairs		
National Infoday and Brokerage – Clean Hydrogen for Europe	ThermWatt. **https://pq-ue.ani.pt/content/eventos/16523_pitch_miguel_c_oliveira.pdf**	2022
PhD Open Days 2022 (Instituto Superior Técnico)	Simultaneous Water and Energy Use Improvement in Process Industry. **https://phdopendays.tecnico.ulisboa.pt/files/sites/144/poster-phd-open-days_miguel-castro-oliveira.pdf**	2022

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List of Code Listings

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List of Abbreviations

Abbreviation	Meaning
AHS	Adsorption heat storage
CAPEX	Capital expenditure
CCS	Carbon capture and storage
CCU	Carbon capture and use
CRC	Clausius-Rankine Cycle
CWEI	Combined Water and Energy Integration
DHW	Domestic hot water
DP	Dynamic programming
EU	European Union
GHG	Greenhouse gases
HDWWT	Heat-driven Wastewater Treatment
HEN	Heat exchanger network
HENG	Hydrogen-enriched natural gas
HR	Heat Recovery
HRSG	Heat recovery steam generator
IPOPT	Interior point optimizer
KPI	Key performance indicators
LP	Linear programming
LTES	Latent thermal energy storage
MD	Membrane Distillation
MED	Multi-effect Distillation
MILP	Mixed-integer linear programming
MINLP	Mixed-integer non-linear programming
MOP	Multi-objective programming
MP	Mathematical programming
MSFD	Multi-stage Flash Distillation
NLP	Non-linear programming
NZLD	Near-zero liquid discharge
PA	Pinch analysis
PI	Process integration
OAT	One-at-a-time
OPEX	Operational expenditure
ORC	Organic Rankine Cycle
PCM	Phase change material
PNUEA	Programa Nacional para o Uso Eficiente da Água

RNC2050	Portugal Roadmap for Carbon Neutrality
SCBC	Supercritical CO_2 Brayton Cycle
STES	Sensible thermal energy storage
TCES	Thermochemical energy storage
TES	Thermal energy storage
TP	Thermal process
TSI	Total Site Integration
TWS	Thermochemical water splitting
WAHEN	Water Allocation and Heat Exchanger Network
WCA	Water cascade analysis
WEIS	Water and Energy Integration Systems
WEN	Water-Energy Network
WENex	Water-Energy Nexus
WHN	Water-Heat Nexus
WHR	Waste heat recovery
WP	Water-using process
WPA	Water pinch analysis
WR	Water recirculation
WtE	Waste-to-energy
WWtE	Wastewater-to-energy
ZLD	Zero-liquid discharge

Nomenclature

Symbol	Description	Unit
A	Heat exchanger area	m^2
AF	Air-to-fuel ratio	kg/kg
ARD	Average relative deviation	None
C	Concentration of a contaminant in a water stream	kg/m^3
C_P	Specific Heat Capacity	J/(ºC.kg)
CAPEX	Capital expenditure	€
$CO_{2,eq}$	Annual equivalent carbon dioxide emissions	kg $CO_{2,eq}$/ year
DW	Annual discharge water quantity	m^3/year
DWFW	Discharge Water to Freshwater Ratio	None
eff	Yield/ Efficiency	None
EcoEff	Aggregated eco-efficiency	€/kg $CO_{2,eq}$
EC	Annual final energy consumption in a plant	J/year
EF	Equivalent carbon dioxide emission factor	kg $CO_{2,eq}$/J
EGHGF	Energy carbon footprint	kg $CO_{2,eq}$/J
Elec	Generated electricity	W
ElecC	Annual electric energy consumption	J/year
EWS	Annual hot and cold utility consumption in a water system	J/year
EWSR	Energy in Water System in the Improved Scenario over the Baseline Scenario	None
FC	Annual fuel consumption	J/year
FW	Annual water consumption	m^3/year
GHGI	Greenhouse gas emissions intensity	kg $CO_{2,eq}$/ kg Prod
h	Specific enthalpy	J/kg
H	Enthalpy	J
LHV	Fuel lower heating value	J/kg
M	Mass flow rate	kg/s
OBJ	Objective-function of the dynamic programming problem over unit of time	€/s
OBJEff	Objective-function of the dynamic programming problem	€
p	Pressure	Pa
PB	Payback period/ Payback time	years
PM	Molecular mass	kg/mol
PMP	Produced material productivity	€/kg Prod
Price	Unitary price	€/m^3 and €/J

Prod	Annual production in a plant	kg Prod/ year
q	Allocated enthalpy	W
r	Radius	m
$\mathbf{Red.CO_{2,eq}}$	Annual absolute reduction of equivalent carbon dioxide emissions	kg $CO_{2,eq}$/ year
Revenue	Annual revenue/ sales turnover in a plant	€/year
RH	Annual total quantity of recirculated heat in a plant	J/year
RHEB	Recirculated Heat to Baseline Total Energy Ratio	None
RHFTP	Recirculated Heat to Baseline Fuel Used in Combustion-based Processes Ratio	None
RTW	Annual quantity of recirculated treated water	m^3/year
RTWTW	Recirculated to Produced Treated Water Ratio	None
RTWWSav	Recirculated Treated Water to Water Savings	None
Sav	Annual monetary savings	€/year
SElecC	Specific electric energy consumption	J/kg Prod.
SFC	Specific fuel consumption	J/kg Prod.
SFW	Specific water consumption	m^3/kg Prod.
t	Time	s
T	Temperature	ºC
TW	Annual treated water production	m^3/year
TWWW	Treated water to Wastewater Ratio	None
U	Overall heat transfer coefficient	W/(m^2.ºC)
wEWS	Annual withdrawn quantity of consumed hot and cold utilities in a water system	J/year
wEWEWS	Withdrawn Energy from the Water System in the Improved Scenario over Energy in the Water System in the Baseline Scenario	J/year
WEF	Water energy footprint	J/m^3
WH	Annual total quantity of waste heat and heat losses in a plant	J/year
WHE	Waste Heat to Total Energy Ratio	None
WHFTP	Waste Heat to Natural Gas Used in Combustion-based Processes Ratio	None
WW	Annual wastewater production	m^3/year
Y	Concentration of a gas component	None
$\boldsymbol{\alpha}$	Thermal diffusivity	m^2/s
$\boldsymbol{\rho}$	Density	kg/m^3
$\boldsymbol{\tau}$	Temperature constant associated to phase change material microstructure	ºC

Greek Letters

Symbol	Description
α	Thermal diffusivity
Δ	Variation
η	Efficiency
ρ	Density
τ	Temperature constant associated to phase change material microstructure

Subscripts

Symbol	Description
additional	Additional
app	Apparent
Air	Air stream
Amb Air	Ambient air stream
Baseline	Baseline case of a plant (a Water and Energy Integration System has yet to be implemented)
Ceramic	Produced ceramic material stream
cont.	Contaminant present in a water stream
conversion	Energy conversion
C. Air	Combustion Air Stream
Cold	Cold Fluid Stream
CombGas	Gas stream resulting from combustion chamber
Cond	Condenser
Concentrate	Concentrate stream at the outlet of a Multi-effect distillation unit
Cooler	Water System Cooler
Cool	Cooling fluid stream
Cool. Air	Cooling air stream
Cool. Ut.	Cold Utility
exp	Experimental value
ext	External
Econ	Economiser
Eff	Effective
Eff1	First effect of a Multi-effect distillation unit
Effk	Second-to-last effect of a Multi-effect distillation unit
Electr.	Electrolysis
ES	Energy Source

Evap	Evaporator
Ex	Exhaust Gas Stream
Fuel	Inlet Fuel Stream in a Combustion-based process
FW	Freshwater/ Feed water in a water system
Gas	Heat source gas stream
hydr	Hydraulic
$\mathbf{H_2}$	Hydrogen fuel stream
Heater	Water System Heater
Heating	Stream heating
Hot	Hot Fluid Stream
Hot Air	Heated cooling air stream at the outlet of a ceramic tunnel kiln
Hot. Ut.	Hot Utility
HS	Heat source stream
HT	Heat Transfer
HTF	Heat Transfer Fluid
HRSG	Heat recovery steam generator
in	Inlet
int	Internal
kiln	Ceramic plant kiln
L	Saturated liquid
Losses	Stream losses
mech	Mechanic
med	Logarithmic Mean
mixed	Stream which has been mixed with others
MED	Multi-effect distillation unit
nom	Nominal
NG	Natural gas stream
out	Outlet
Org	Organic fluid stream
ORC	Organic Rankine Cycle unit
Prod	Stream of the material product to be produced in a plant
PCM	Phase change material
reac.	Reaction
recic. stream	Recirculated stream
required	Required energy
Rec Air	Recirculated hot air stream
sim	Simulation value
Sludge	Sludge or concentrate stream resulting as a by-product from

	wastewater treatment
split	Stream that has been divided
Stored	Stored
SuperH.	Superheater
supply	Supplied
to – be – mixed	Stream which is set to be mixed with others
to – be – splitted	Stream which is set to be divided
TP	Combustion-based process
TW	Treated water stream
Unit	Single sub-unit of a heat-driven wastewater treatment unit (effect or stage)
V	Saturated vapour
Vapour	Vapour stream
with	Withdrawn
W	Water Stream
WEIS	Improved Case (a Water and Energy Integration System has been implemented)
WH	Waste heat stream
WP	Water-using process
WSp	Water splitting reaction
WW	Wastewater stream/ Water stream at the inlet of a wastewater treatment unit
WWtE	Wastewater-to-energy/ Energy recovery from water unit
WWT	Wastewater Treatment Unit

Superscripts

Symbol	Description
·	Time-depending derivative
0	Standard reaction

Other Symbols

Symbol	Description
d	Infinitesimal variation
f	Function of Variable

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1. Introduction

Process industry is responsible for a significant part of the total use of final energy in the context energy systems of each region of the world and also for significant levels of water consumption and discharge [1,2]. These are attributed to the use of each one of these categories of resources in energy-using and water-using processes [3]. The significant use of these resources requires the planning and further implementation of improvement measures with the ultimate aim to fulfil the necessary requirements to promote a sustainable development of the production processes [4], as well as the mitigation of social, environmental and economic issues related to the unbalanced utilization of these resources [2].

A commonly proposed and effectively implemented methodology oriented to reduction of resource input through the valorisation of material and energy outputs is the methodology of process integration (PI). Process integration may be regarded as assessment of the set of all process and systems existing in a plant and all potential interdependencies to optimize external resources usage. The research fields of water and heat integration subsists on the application to water and energy use of the principles of process integration [5].

The conceptualization of water recirculation and energy recovery systems (either the simultaneous application of these practices or standalone application of these) overall consists on the application of the principles of water integration and heat integration, which are specific applications of the process integration methodology for the water and energy resources, respectively [6–8]. In practice, and in simple terms, water integration subsists on the principles of water recirculation [9], while heat integration applies the principles of waste heat recovery [10]. A common case of the simultaneous application of these types of practices is in water allocation and heat exchanger networks (WAHEN), which are water systems in which both freshwater and energy utilities consumptions are planned to be reduced [6–8]. In practice, the conceptualization of the systems is based on the use of a water stream as both a to-be-valorised heat stream and for the purpose of reducing the total feed water input on the system [6]. Another approach which involves the simultaneous application of the practices of water recirculation and heat recovery is the installation of heat-driven water treatment technologies, which are set to reduce the total feed water input in a system through the recirculation of treated water with the requirement of a minimized energy input [11].

The study of water and heat integration has the ultimate goal to study potential improvement of water and energy efficiency [8]. The study of energy efficiency has been the scope of the majority of international energy and environmental policies, namely the most recent European 2030 climate & energy framework [12], European Green Deal [13], European 2050 long-term strategy [14] and the Paris Agreement [15]. The interdependencies of water and energy resources, which includes the understanding of the improvement of water use through the understanding of the use of energy, have been studied on the scope of the water-energy nexus [16]. The water and energy integration methodologies may be applied in a high number of industrial processes and also a high number of industrial sectors [8]. The concept of water-energy nexus (WENex) and the methodology of process integration are aligned in the aspect that simultaneous water recirculation and energy recovery systems are possible to be commissioned by the sharing of discharge streams which contain considerable quantities of water and energy that may be furtherly valorised [17,18].

The conceptualization and further on-site implementation of water recirculation and energy recovery systems may require the analysis of the occurring physical phenomena within single unit operations or in the whole plant in a holistic perspective. Industrial processes (namely the ones whose operation in essence requires the supply of significant quantities of water and energy) are the main scope of study of water and energy integration. Several categories of industrial processes may be studied for the conceptualization of water and energy stream recirculation systems, including: Thermal processes (TP) (which include combustion-based processes) [19,20], Water-using processes (WP) [21], Wastewater treatment (WWT) units [22] and Wastewater-to-energy (WWtE) units. While the main object of study of heat integration only are thermal processes [23], water integration approaches systems that include processes which use water as an utility to remove a certain quantity of contaminants and a furtherly installed wastewater treatment unit (being based on the recirculation of the water, wastewater and treated water streams that make part of the system) [6].

The practical implementation of the principles of water and energy integration resides on the exploitation of all possible interdependencies between all (or a significant part of) existing and operating industrial processes. In practice, such implementation is performed by the application of several improvement technologies [24]. On the side of energy efficiency improvement, it is worth emphasizing the application of waste heat recovery (WHR) technologies [10,25], which are set to allow the most possible rationalization of thermal energy within a plant, and, for instance, encompass thermal energy storage (TES) [26,27], in the case of dynamic energy demands. On the side of water efficiency improvement, it is worth emphasizing the application of wastewater treatment (WWT) technologies [28], which allow the removal of contaminant present in wastewater streams which are then potentially recirculated as additional water inputs. In an even further exploitation of the state-of-the-art technologies, it is worth emphasizing the role of waste-to-energy (WtE) for the generation of additional primary energy (fuels) input on combustion-based processes, in which are encompassed technologies for energy recovery from wastewater [29]. The effective implementation of the aforementioned technologies results on the transformation of open-loop systems (with a linear economy character) to closed-loop systems (with a circular economy character) [30], which encompass the recirculation of water and heat source streams from some processes to others in an optimised manner.

The analysis of the operation of industrial processes, whether in a standalone perspective or, rather, on the context of a plant or within the operation of water recirculation and energy recovery systems, may be performed by the development of computer models [31]. These models are set to allow the assessment of specific conditions associated to the operation of industrial processes and the systems encompassing the sharing of streams from these processes [16,32]. The main technical purpose for such development effort is the assembling of simulation and optimisation models for plants (or rather sections of plants which encompass a multitude of intensive water and energy processes, whose interdependencies may be exploited for the promotion of resource efficiency). Ultimately, these models are set to analyse potential overall benefits in terms of water and energy use, which in a post-processing perspective may be expressed throughout the determination of key performance indicators (KPI) associated to eco-efficiency and circular economy character promotion.

This work approaches the concept of Water and Energy Integration Systems (WEIS), which may be defined as complex installations to be installed in end-use sector facilities set to perform the maximum use of the recirculation of waste heat and water streams for the purpose of causing an overall eco-efficiency promotion (by the conjoined effect of energy efficiency improvement, freshwater use reduction and solid/ gas contaminant emissions reduction), using a set of technologies that may be used in the context of the exploitation of the interdependencies of energy and water resources [33]. It is both an advancement and a generalization of the closed-loop system types also mentioned above and is set to be implemented for all facilities in which combustion-based processes and water-using units are present, and as such it may be implemented in the multitude of sectors which are encompassed by the overall sector of process industry (being the example of the sectors of Iron & Steel, Non-ferrous metals, Cement & Lime, Ceramic, Glass, Paper & pulp, Textile, Chemical Processes and Food, Beverage & Tobacco).

1.1. Motivation

The aims of the PhD thesis are generally in accordance with the objectives of the most recent energy and environmental policies of the European Union, namely: 2030 climate & energy framework [12], 2050 long-term strategy [14] and European Green Deal [34]. Additionally, it is also aligned with the aims of the Paris Agreement, namely on the mitigation of the impacts of climate change and the goal of the agreement to limit global warming below 2 ºC (and preferably 1.5 ºC) [35]. In a perspective of the current socio-economic situation, this work may be a significant contribution to the development of a potential approach for the mitigation of overall impacts related to the economic crisis provoked by the COVID19 pandemic [36] and the Russia-Ukraine War [37]. In this prospect, and in a further perspective, it may constitute a contribution to an overall solution for the socio-economic issues related to the global energy crisis and water scarcity phenomena that have been prominent in the course of 2022 – 2023.

In specific, it is aligned with the three pillars constituting the EU strategy for energy system integration [38]:

- The first pillar dealing with the Energy Efficiency and Circular Economy Nexus, namely in respect to the performance of waste heat recovery and energy recovery from wastewater;
- The second pillar dealing with the Renewable-based Electrification, namely in respect to the performance of electricity generation through waste heat recovery;
- The third pillar dealing with Alternative low-carbon fuels, namely in respect to the practice of

green hydrogen production.

1.2. Knowledge Gaps

The problem of water and energy efficiency improvement has been approached with the use of several computational methods, which may then be used to build models whose results may be replicated in real-life industrial sites. While the improvement of energy efficiency has been achieved by the application of several heat recovery (HR) technologies and strategies, the improvement of water efficiency subsists on the assessment of potential water recirculation (WR) points within a system containing a certain number of water-using processes and wastewater treatment units. The process integration methodology has been widely applied for the solving of these problems, being highlighted the use of the heat pinch analysis method for the improvement of thermal energy use [39–41] and the water pinch analysis for the improvement of water use [42,43]. In respect to the latter, an approach designated as Combined Water and Energy Integration (CWEI) has been implemented for the assessment of the use of recirculated water streams as simultaneously additional water and heat sources [6,44]. Furthermore, an approach which aims to be applied for the inclusion of the highest number of processes (in the limit, all the processes in a plant) designated as Total Site Integration (TSI) has been developed subsisting on the notion of a common utility systems for a set of energy-using processes and the further identification of heating and cooling requirements (hot and cold utilities) [45–53].

Overall, the implementation of the aforementioned methodologies (either in on the perspective of running of numerical models and in real-life plants) are characterized by the following knowledge gaps:

- Only a limited number of technologies have been considered and implemented for each conceptualized system (which is the case of heat exchanger networks for HR, wastewater treatment for WR and CWEI and an ensemble of heat exchanger networks, electricity generation components and thermal energy storage for TSI);
- The methodologies are overall one-dimensional in respect to the type of industrial processes being considered (this is, only approaching energy consumers or water consumers), and do not analyse all the potential interdependencies between processes which are implemented for different operational ends and consume different utilities;
- In the context of industrial implementation, energy efficiency improvement-related measures have been given priority in comparison to water efficiency improvement.

1.3. Original Contributions

The main original contribution of this work is the development of a customised simulation and optimisation tool designated ThermWatt. The ThermWatt tool has been in development since 2019 and emerged in the scope of the works performed for the Portugal2020 research project

EcoTermIP [54] and the R&Di activities performed by ISQ – Instituto de Soldadura e Qualidade. Since 2019, new developments have been added to ThermWatt, which has become an internal initiative within the R&Di department of ISQ. National and international R&D projects in which ThermWatt has been used for its planned purposes (and in this prospect receiving updates owing to the specific modelling requirements associated to these) include GreenH_2Atlantic, BIOMAC and several projects within *Agendas Mobilizadoras para a Inovação Empresarial* (developed in the scope of the Recovery and Resilience Plan (RRP) created by the Portuguese government).

ThermWatt consists mainly of a Modelica simulation module, designated as ThermWatt Library. Nonetheless, other software packages have been implemented for the overall development of ThermWatt, namely the Python language for the development of steady state-based optimisation models.

The overall work performed for this thesis secondarily converges on the development of new water and energy integration concepts to be in practice implemented in grassroot or existing process industry plants. These are new generalized superstructure conceptualizations to be adapted and implemented for each individual industrial case, and encompass the implementation of technologies for heat recovery, thermal energy storage (in the case of dynamic systems), wastewater treatment and energy recovery from wastewater.

1.4. Specific Objectives

The objectives of the present PhD thesis subsist simultaneously on the achievement of benefits related to eco-efficiency promotion (either at the levels of plants, process industry sectors or countries) and the development of a computational tool for the implementation of Water and Energy Integration Systems (WEIS). In this sense, in relation to the first point, the specific objectives of this work are:

- Establishment of the concept of Water and Energy Integration Systems (WEIS), which aims to surpass the drawbacks associated to the most complex methodologies (CWEI and TSI), considering all potential interdependencies between energy and water-using processes in a plant and the implementation of several technologies;
    - Establishment of WEIS configurations which may be implemented (in the limit) to all the plants of the process industry containing a determinate number of thermal processes and water-using processes;
    - Development of several scenarios within the scope of these configurations which subsist on different levels of water and heat recirculation and the implementation of different analogous technologies;
- Assessment of the sustainability promotion, through a primary economic and environmental viability assessment and a further assessment based on the estimation of several eco-efficiency, circular economy character and sustainability policies compliance indicators.

In relation to the latter point, the specific objectives of this work are:

- Development of reusable computational models encompassing the assembling of the flowsheets of the WEIS configurations, and which overall are set for scenario analyses and optimisation procedures;
- Development of a computational tool for several representatives of academia, industry and enterprises, which may be used or rather adapted for the achievement (in a basis of virtual reality) of similar results for other industrial sites.

1.5. Thesis Outline

The present thesis is organized in the following way (excluding the present Chapter 1):

- Chapter 2 presents a comprehensive literature review regarding all the aspects for the implementation of Water and Energy Integration Systems (WEIS) in process industries (which includes the exploitation of improvement technologies and the contextualization of the benefits generated by water efficiency improvement, energy efficiency improvement and environmental impact mitigation) and the existing simulation and optimisation models for these systems, as well as the conceptualization of generalized superstructures for these systems based on the overall knowledge exploited in literature;
- Chapter 3 presents a description of the proposed methodology and the aspects related to the development of component-level models;
- Chapter 4 presents the system-level simulation models developed for two process industry case-studies, encompassing the general description of each case-study (baseline scenarios), proposal of WEIS configurations, simulation results and scenario analyses. The two case-studies are inserted within the Portuguese ceramic industry. While case-study 1 is analysed on the basis of continuous processes and a steady-state perspective, case-study 2 is analysed on the basis of a combination between continuous and batch process and a transient-state perspective;
- Chapter 5 presents the optimisation procedure taken with the aim to assess potential improvements at the level of water use, energy use and environmental impact mitigation in plants, presenting the developed optimisation models developed with the Modelica and Python languages for each specific case-study and the results obtained for several key performance indicators in respect to the economic and environmental impact-related performance;
- Chapter 6 presents a final assessment based on the determination of key performance indicators for the assessment of the aspect related to eco-efficiency, circular economy potential and strategic objectives potentials subsisting on the results obtained for the approached case-studies;
- Chapter 7 presents the conclusions and future work proposal in respect to the whole work.

2. Literature Review and Background

The present chapter aims to present a complete framework of the theoretical scientific aspects associated to the research on Industrial Processes, Water and Energy Integration and the development of models for simulation and optimisation for systems installed in process industry plants. It is also set to explore the societal aspects associated to the overall promotion of industrial sustainability associated to Water and Energy Integration implementations in plants, which in practice it is performed by establishing the framework of Water and Energy Integration in the promotion of low carbon and circular economies, the most recent energy and environmental policies and within the different industrial sectors and regions of the globe. In this prospect, this chapter subsists on the performance of a literature review for the establishment of the overview of the implementation of water efficiency, energy efficiency and related sustainability practices in process industries and the state-of-the-art related to the planning, conceptualization and installation of systems encompassing several levels of water treatment, water recirculation and energy recovery.

A set of scientific publications by the authors about this subject [55–57] were developed having as a basis the specific content present in this section.

2.1. Strategic Framework

Water efficiency and energy efficiency are concepts that have been gradually introduced in the energies policies adopted by each country in the world. In the European Union, targets for an efficient water and energy use were, respectively, established in the 2000 Water Framework Directive [58] and the 2012 Energy Efficiency Directive (namely its 2018 Amendment [59]). In a wider perspective, the most relevant objectives of EU regarding sustainability have been established in the most recent 2030 climate and energy framework (up to 40 % reduction of GHG emissions from 1990 levels, 32 % share for renewable energy and 32.5 % energy efficiency improvement) [60]. The EU have been even further beyond advancing on the concept of sustainable development with the introduction of the European Green Deal. This deal was introduced as a roadmap encompassing actions aiming to boost resource efficiency through moving economic activities to a circular economy, and also to restore biodiversity and reduce pollution [13].

2.1.1. Framework of Low Carbon and Circular Economies Promotion

The principle of progress towards industrial sustainability is based on the reduction of resource consumption and the environmental impacts associated to the waste produced in plants [61]. The most important resources include water, electric energy, fuels and process raw materials. In practice, promotion of industrial sustainability may be performed by the implementation of improvement measures which overall optimise water and energy use [62,63], the application of renewable energy resources [64] and the application of waste-to-energy technologies [65]. The concept of circular economy has been emerging on the scope to transform waste into potential by-products, promoting reuse, recovery and recycling, in which the life cycles of the production chains are optimised [66]. In the limit, the application of several measures converges on the reuse of resources (either material or energy) within the same industrial site. In respect to the recirculation of matter and energy within a system, the scheme presented in Figure 2.1 represents in a generic form all the material and energy flows in a perspective of circular economy.

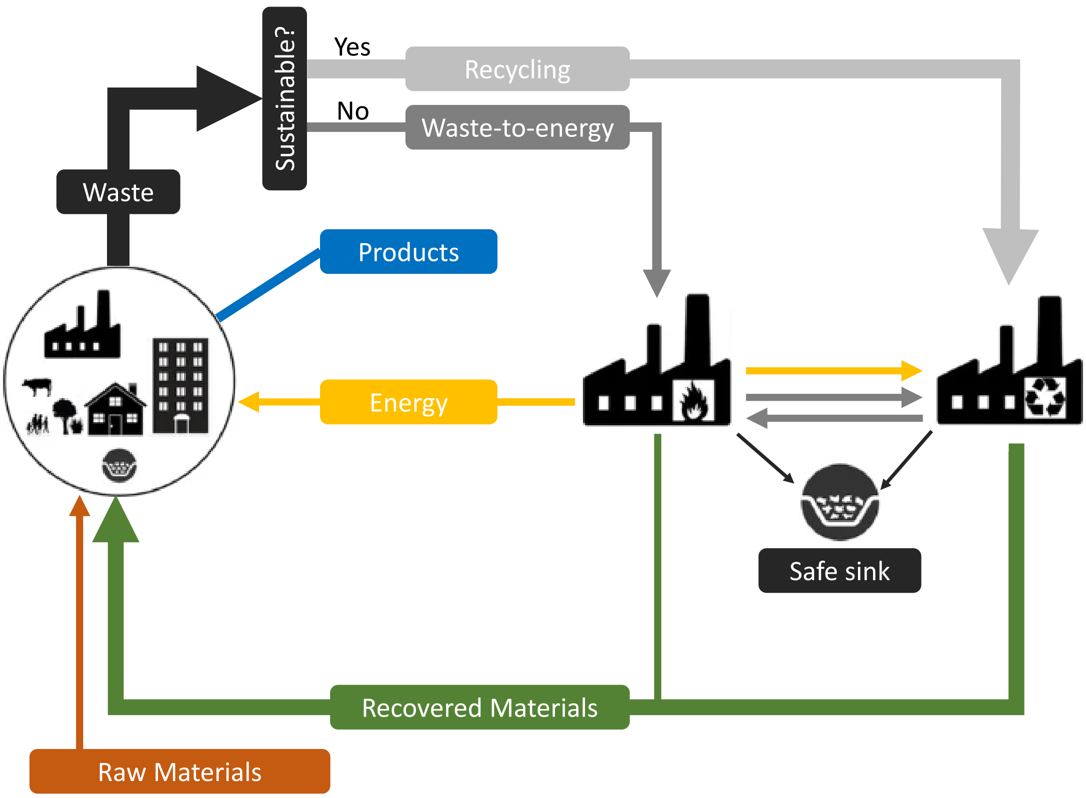


Figure 2.1. Recovery of energy and material streams in a perspective of circular economy (adapted from [67])

The scheme presented in Figure 2.1 may be re-interpreted in terms of the flows of water and thermal energy in a manufacturing industry plant, as these are specific flows encompassed by respectively the generic matter and energy flows present in the scheme. Setting off from the waste generated from a plant, it is to note that this waste may be:

- Not only interpreted as material waste, such as the one present in wastewater [68];
- But also as thermal energy that is lost in processes such as combustion (waste heat) [69].

The streams with considerable waste heat potential may be recycled to the energy-using process within a plant (such as combustion-based processes), serving as additional heat sources which enable the opportunity to save on the consumption of the primary energy source (fuel) [63]. In this prospect, the waste heat contained in these streams will constitute a part of the total supplied energy which will be converted into available energy to the operations of the plant [63].

The wastewater streams must be pass through a treatment system to enable a sustainable recirculation. From the water treatment systems, it results two streams:

- Treated water streams that may constitute recovered materials useful for the overall improvement of the operation of the plant (in these case for the generation of savings in freshwater consumption) [70];
- Sludge streams that may be valorised through the implementation of waste-to-energy technologies [71]. A part of the total quantity of discharge water may also be valorised in terms of energy recovery (for instance, in the case of hydrogen production units [72,73]).

The re-interpretation of the scheme of Figure 2.1 considering the aforementioned aspects is presented in Figure 2.2.

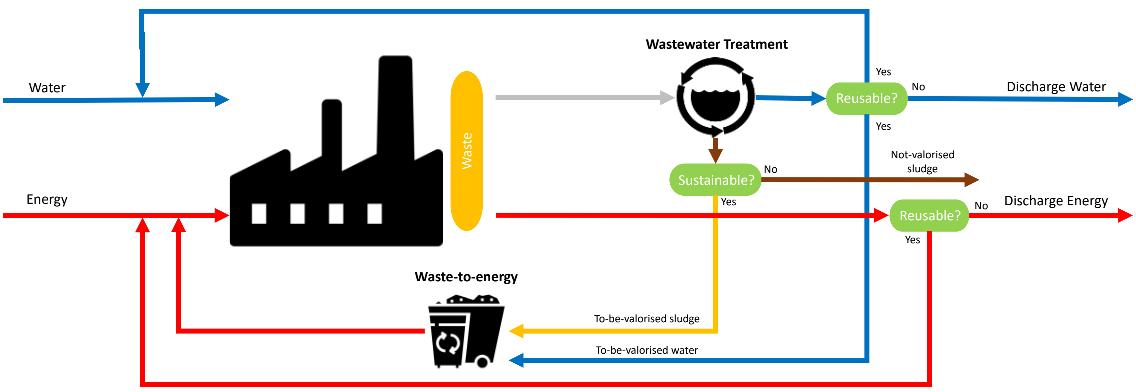


Figure 2.2. Re-interpretation of the Circular economy scheme for water and energy recirculation

2.1.2. Framework of the Energy System Integration Strategy

The scope of this thesis is mainly directed to the European Union's Energy System Integration Strategy, dealing with the practical application of the aims of this strategy on several industrial sectors. The Energy System Integration Strategy itself resulted from the combination of the aims of both the European Green Deal [74] and the 2050 long-term strategy [75], in the sense that it pretends the attainment of a net-zero GHG emission-based economy through the promotion of the circular economy perspective on the conceptualization and operation of energy systems.

In the context of the opportunities related to the energy system and water resources supply systems of Portugal, the Roadmap for Carbon Neutrality 2050 (RNC2050) [76] and the *Programa Nacional para o Uso Eficiente da Água* (PNUEA) [77] have been proposed as guiding instruments. These two strategies are based on the delineation of specific objectives for all the end-use sectors, with RNC2050 containing specific guides for a set of subsectors of the whole industrial sector.

The definition of guiding principles and the contextualization associated to each pillar of the EU Energy System Integration Strategy on the practical work inherent to this thesis is presented in Table 2-1.

Table 2-1. Framework of water and energy efficiency in each industrial sector

Pillar	Framework	
1st Pillar Energy Efficiency and Circular Economy Nexus	Definition of Guiding Principles	• Energy efficiency-first principle (giving priority to energy demand-side solutions in relation to energy supply-side ones, in the case that these are more cost-effective); • Waste heat recovery from industrial sites at the centre of intra-plant energy efficiency improvement and the functioning of district heating and cooling networks (which is based on the promotion of WHR practices in a wider perspective and the surpassing of existing barriers); • Energy recovery from wastewater (mainly through the production of biofuels).
	Contextualization	• This work is focused on the improvement of energy efficiency (as well as water efficiency through the promotion of the recirculation of water and energy stream which may be further valorised; • The recirculation of these streams allows the conceptualization of systems encompassing industrial processes which are circular in nature (resources inevitably produce wastes as by-products which are in its turn recirculated as additional resources); • The main focus is heat recovery and water valorisation (either as feed water, waste heat streams or through further valorisation in waste-to-energy).
2nd Pillar Renewable-based Electrification	Definition of Guiding Principles	• Compensation of growing electricity demand through the promotion of the use of renewable energy resources as primary energy forms; • Electrification of industrial processes; • Application of energy storage technologies.
	Contextualization	• The electrification of end-use sectors (in this case, industry) is potentially achieved through the application electricity-producing heat recovery-based thermodynamic cycles, which is also inserted within the scope of this work.
3rd Pillar Alternative low-carbon fuels	Definition of Guiding Principles	• Promotion of the use of green hydrogen on sectors with more difficult decarbonisation; • Promotion of carbon capture and storage (CCS) and carbon capture and use (CCU).
	Contextualization	• The application of waste-to-energy to the sludge from wastewater treatment units may result on the production of renewable biofuels (for instance, through anaerobic digestion) and hydrogen (for instance, through electrolysis).

As may be observed by analysing the information in Table 2-1, the overall scope of this thesis essentially meets the objectives of the 1st Pillar of the EU Energy System Integration Strategy. The work inherent to the thesis is set to assess an overall potential water and energy efficiency improvement in a plant through the application of the principles of heat recovery and energy recovery from wastewater. In relation to the latter aspect, it is to note that such energy recovery measures are based on both the use of wastewater streams as heat source streams and in the sense that the sludge resulting from wastewater treatment units is set to be furtherly valorised, as clarified in Table 2-1.

2.2. Research Opportunities and Knowledge Gap

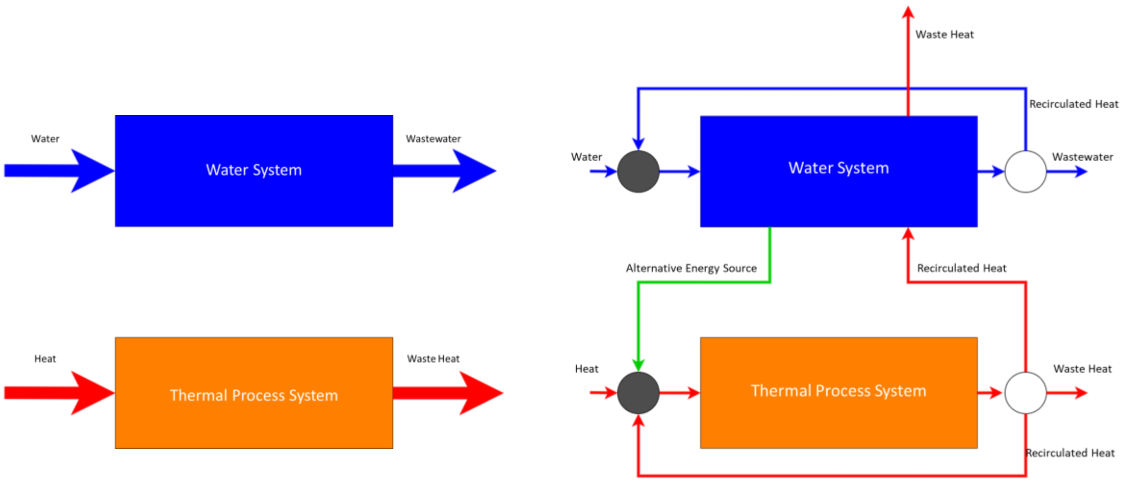
The scope of the research regarding Water and Energy Integration subsists on the existing research on water treatment, waste heat recovery and environmental impact assessment in relation to water pollutant and GHG emissions, as well as the industry-based knowledge and effective implementation of water and energy efficiency improvement practices. In literature, several authors have been identifying the gaps on the research associated to either water treatment and recirculation or waste heat recovery, as well as Combined Water and Energy Integration. Although the literature gap in relation to water treatment and recirculation and WHR is not significant, the field of Combined Water and Energy Integration is not associated to the same level of exploitation by researchers. The production of theoretical studies within this field would assist on the filling of this research gap. As may be logically deduced, the knowledge gap in terms of industry application is significantly higher, as it deals with the effective handling of water and energy efficiency improvement measures in practice. In Table 2-2, it is characterized the knowledge gap inherent to Water and Energy Integration in terms of academic, industrial and enterprise-based applications.

Table 2-2. Characterization of Knowledge Gap

Type	Characterization	Ref.
Academic-side Gap	In respect to WHR technologies and strategies: • Coupling of existing WHR technologies with thermal energy storage technologies (in specific PCM-based storage). In respect to industrial system conceptualization in general: • Consideration of water and heat losses on model development; • Consideration of different options of wastewater treatment technologies for the conceptualization of superstructures for water systems; • Use of sensitivity analysis tools for the consideration of variance associated to determinate parameters. In respect to specific modelling and optimisation methods: • Use of the multi-objective programming methodology for the optimisation of water and energy use in industrial sites; • Use of dynamic models (in general) to account for daily cycles, multiperiod approaches and long-horizon operations.	[78,79]
Industrial-side Gap	In respect to the general use of water and energy in industry: • Preference of industrial stakeholders for energy-related issues rather than water-related issues • Higher availability of energy-related data in relation to water-related data	[80]
Enterprise-side Gap	• Supply of freeware tools for the assessment of several process integration scenarios; • Development of dynamic-based and control-based simulation tools incorporating online optimisation systems; • Extension of existing simulation tools for different applications.	[81,82]

2.3. Process Integration and Water-Energy Nexus within Process Industries

The effective attainment of results on water and energy efficiency improvement in a plant must subsist on the conceptualization of the retrofitted system passing by the planning of the recirculation of water streams and streams containing reusable waste heat from one process to several other processes [18]. These systems include a set of industrial processes within a plant in which it is priorly identified that such type of water and energy efficiency improvement measures are possible to be implemented and that such implementation brings benefits at the level of cost and environmental impact mitigation. These systems are operationally set to include a defined number of water-using processes and a defined number of thermal processes and are inherent to the overall energy system of a plant, encompassing its energy supplies (fuels and utilities) and energy demands (at the level of useful energy). These systems are circular economy-based and overall allow decreased levels of water and energy consumption and the mitigation of overall GHG emissions and contaminants existing in wastewater. The most generalist conceptualization of these systems and its comparison with linear economy-based systems is represented in Figure 2.3.



a) b)

Figure 2.3. General scheme for a) a linear economy-based industrial installation constituted by a water system and a thermal process system and b) a refurbished circular economy-based overall system constituted by a water system and a thermal process system (black-filled circles (●) represent stream mixing, while unfilled circles (○) represent stream splitting)

In literature, the types of possible to be conceptualized closed-loop systems for waste heat and water stream recirculation take the following designations:

- Heat exchanger networks (HEN) (for heat exchanger installation-based heat recovery);
- Near-zero liquid discharge (NZLD) (for water systems with significantly decreased wastewater discharge owing to water treatment and recirculation);

- Water-Energy Networks (WEN) and Water Allocation and Heat Exchanger Networks (WAHEN) (for water systems in which previously discharged water streams are recirculated to simultaneously decrease the use of freshwater and hot and cold utilities).

As may be verified, each one of the aforementioned systems are set to encompass only a limited part of the existing processes in a plant (either the combustion-based processes or units belonging to a water system in a standalone perspective). The full exploitation of the interdependencies between water and energy resources within a plant (as summarily schematized in Figure 2.3) shall subsist on a more embracing concept, which is furtherly introduced in the chapter 3 of this work.

2.3.1. Basic Concepts of Heat Recovery

The conceptualization of waste heat recovery (WHR) systems subsists on the application of energy management principles to plan the installation of several technologies requiring and promoting the recirculation of streams with an associated waste heat potential so to obtain savings in fuel consumption or electric energy consumption [83,84]. In this prospect, a heat recovery system may be planned considering the following opportunities:

- Reduction of fuel use in the combustion-based process from which the waste heat stream is emitted [84];
- Reduction of fuel use in other combustion processes [63];
- Reduction of electric energy use by the implementation of a thermodynamic cycle to produce electric energy from a waste heat stream [83].

In the conceptualization of a heat recovery system, additional energy sources may also be included, which in this case represent:

- Thermal energy that is generated by renewable energy integration (such as solar thermal [26]);
- Thermal energy supplied by a thermal energy storage (TES) unit [26,27];
- Waste-to-energy technologies integration [85].

Within these opportunities for additional energy supply, thermal energy storage may reveal as a particularly attractive set of technologies, considering its potential to surpass limitations associated to WHR such as techno-economic issues related to the implementation of conventional WHR technologies and the temporal and/ or geographical mismatch between the additional energy release and supply. In the context of a plant, the required thermal energy to be supplied to a thermal energy storage system may be either supplied by industrial waste heat or the heat from solar thermal collectors [86].

The general conceptualization of a heat recovery system is represented in Figure 2.4.

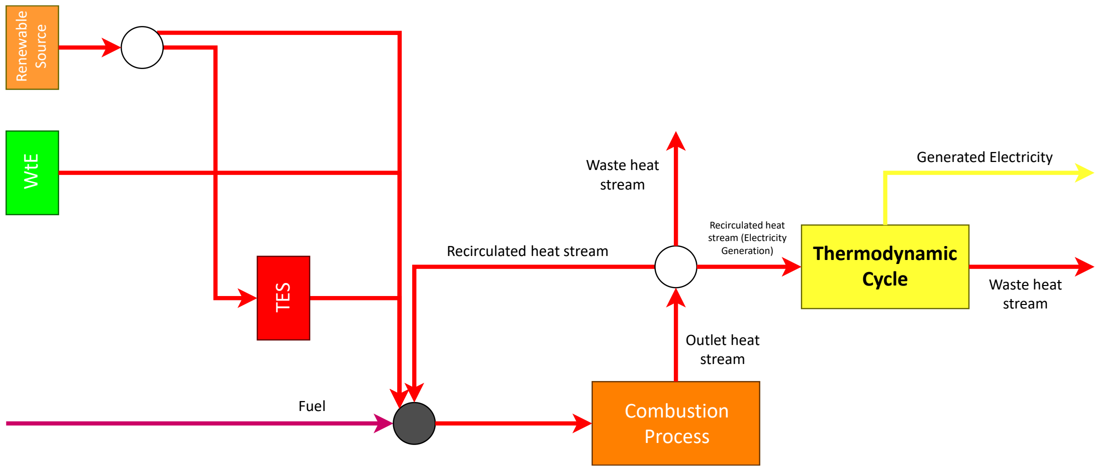


Figure 2.4. Basic approach of a heat recovery system for a combustion-based process considering the recycling of waste streams and the input of additional energy streams

2.3.2. Basic Concepts of Water Recirculation

The recirculation of water streams has a similar principle to the one of heat recovery, in which the water stream at the outlet of a certain process is recirculated in order to produce savings on freshwater consumption [9]. Nonetheless, in the case of the planning of a water recirculation system, it is generally necessary to first treat the wastewater from a determinate process in order to recirculate it [28]. In this sense, these retrofitted systems are referred in this work as water treatment and recirculation systems. In the context of the more complex conceptual simultaneous water recirculation and energy recovery systems, these will be simply referred as water systems, for a reason of convenience. As mentioned afore, a designation used by authors for water systems which are conceptualized to achieve an almost non-existing discharge is near-zero liquid discharge (NZLD) systems [87,88]. Since a complete non-existing discharge is difficult, the term near-zero discharge systems is used instead of zero liquid discharge [89].

In this work, water recirculation is used as a term to encompass both water recycling and water reuse, attending that at the viewpoint of process integration both terms have different meanings [90], with recycling referring the transport of treated water to the initial water-using process and reuse the transport of other to other water-using processes. Taking into account this aspect, the most basic water recirculation approach in this work is based on the recirculation of the treated water stream at the outlet of a wastewater treatment unit, which may be:

- Recirculated to the initial process (Water recycling);
- Recirculated to other processes (Water reuse).

In the context of the conceptualization of water allocation and heat exchanger networks (WAHEN) (which are systems in which energy-using units are present and in whose associated energy consumption is set to be reduced in addition to freshwater), other points of stream recirculation may exist, such as the streams at the outlet of heaters, cooler and the water-using process itself (these streams are set to be recirculated whereas limiting contaminant concentration in determinate points of the water system are not surpassed) [6–8,44,91–113]. In its turn, the discharge streams from the water system (either the discharge water stream from the main water-using line or the sludge stream resulting as a by-product from the wastewater treatment unit) may be furtherly valorised in a context of recovery, through the installation of waste-to-energy (WtE) technologies [85].

The detailed water recirculation approach is pictorially represented in Figure 2.5.

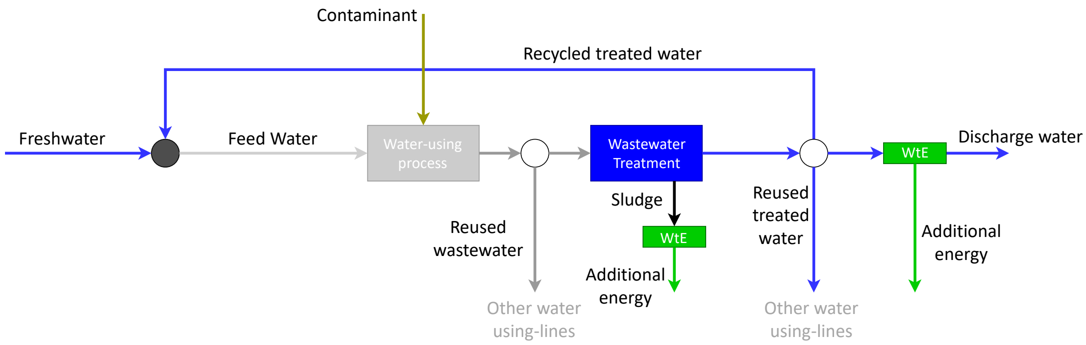


Figure 2.5. Basic approach of a water treatment and recirculation system (representing a single water-using line constituted by one water-using process, one wastewater treatment unit and two wastewater-to-energy units for, respectively, the sludge stream and the discharge water stream)

It is to note that for the conceptual development of water recirculation and energy recovery systems in the context of this work, the following concepts are regarded as analogous:

- **Wastewater treatment** and **desalination** (in this case, desalination represents a specific wastewater treatment unit in which the contaminants are salts);
- **Treated water** and **desalinated water** stream (in the case of desalination units, the set-to-be produced stream is a water stream with a significant quantity of salts removed);
- **Sludge** and **concentrate** stream (in the case of desalination units, the by-product stream corresponding to sludge is the concentrate, in which the removed salts are retained);
- **Wastewater-to-energy** and **energy recovery from water** (in the case of the former term, wastewater designates all types of discharge streams from a water system which may be valorised in terms of energy recovery);

2.3.3. Overview of Process Integration and System Retrofitting

Process integration is a concept essentially used within the field of chemical engineering and used to improve energy efficiency in chemical process industries, such as the petrochemical industry [114]. The application of process integration is nonetheless not only summed up to that area of study or a specific set of industries. In analytical studies, process integration has been applied through the performance of pinch analysis, which is the most commonly applied PI method [115]. Pinch technology may be applied to either mass (mass pinch) [116] or energy (energy pinch, also recognized as heat integration) [117]. In respect to mass pinch analysis, a sub-field of study is water pinch analysis (WPA) [118]. In respect to water integration in particular, several other methodologies are presented in the literature, such as water cascade analysis (WPA) [119]. By virtue of the interdependencies of water and energy use, a concept which approach the application of process integration for the optimization of the use of both these resources has been emerging, known as Combined Water-Energy Integration (CWEI) [6]. In Table 2-3, it is presented a summary of the progress on studies of Water and Energy Integration in the industrial sector.

Table 2-3. Progress on each aspect of interest regarding Water and Energy Integration

Aspect	Progress	Ref.
Overview of Process Integration	Framework of process integration within the improvement of the use of utilities in industry and the involvement of numerical methods, including: • Involvement of mathematical programming, numerical modelling and multi-objective optimisation; • Directions of the implementation of process integration; • Attainment of general results on water savings, energy savings and reduction of environmental impacts.	[120–127]
Pinch Technology for Energy Efficiency Improvement	Application of pinch analysis-based heat integration in industry, including: • Assembling of heat exchanger networks (HEN) in a plant; • Application of pinch technology to improve the operation of industrial processes and systems (for instance, ORC and Kalina cycle); • Simultaneous application of pinch and exergy analysis methods; • Implementation of algorithms for the assembling of energy management scenarios.	[40,80,111–120,103,121,104–110]
Water Minimisation and Recirculation	Implementation of strategies for the minimisation of freshwater consumption and reduction of water footprint, through: • The application of water pinch analysis (WPA) and water cascade analysis (WCA) methods; • Study of water management strategies; • Study of the reduction of wastewater discharge.	[42,88,129,94,122–128]
Simultaneous Water and Energy Integration	More complex research on the simultaneous application of water and energy integration, passing by: • Simultaneous application of water and energy pinch in the context of a water system (Combined Water and Energy Integration); • Application of the concept of water-energy nexus on a process-based perspective.	[16,62,78,130–134]

2.4. Water and Energy Efficiency Improvement Technologies and Strategies

The planning of systems encompassing overall water treatment, water recirculation and energy recovery highly depends on the study of industrial processes and the specific operational conditions associated to these but prominently on the technologies used to valorise water and energy, as well as state-of-the-art strategies for the recirculation of these resources. In the case of water recirculation, the application of wastewater treatment technologies is frequently necessary, as the recirculation of wastewater streams highly limits the recirculation potential. In the case of heat source stream recirculation, it is known the existence of technologies that allow the direct use of determinate streams, although much of the exploited technologies subsist on the use of heat exchanging units.

In Table 2-4, each category of improvement technologies is characterized in a general perspective. In the sequence of Tables 2.5 – 2.10, it is performed a characterization of a set of technologies for each category. In the sequence of Figures 2.6 – 2.12, the characterized technologies are pictorially presented.

Table 2-4. Overall characterization of improvement technologies

Category		Characterization
Heat Recovery (HR)		The basic principle of WHR is the recapture of energy from a material stream generated in a production process to be transported back into the system either as an additional heat source [24] or to produce electric power [84]; Taking into account these two basic energy demand types, several WHR technologies encompassing improved combustion systems, heat exchangers and electricity generation systems have been studied by several authors [10,159].
Thermal Energy Storage (TES)		The existing heat recovery technologies are associated to certain limitations at the level of the significant distance between the heat source and the heat sink, the lack of identification of existing heat sinks and operation disturbances; Being a specific type of HR technologies, thermal energy storage (TES) technologies are set to be implemented for dynamic heat supply and demand levels in a plant, with associated advantages as better capacity factors, avoidance of heat losses and reduced investment cost (in combination with cost expensive components); The TES technologies may be decoupled into sensible (STES), latent (LTES) and thermochemical energy storage (TCES).
	Thermochemical Energy Storage (TCES)	These are a set of technologies which combine both the principles of thermal and chemical energy storage; The existing technologies may be classified into sorption technologies (based on the phenomena of absorption or adsorption) and chemical reaction technologies (which involve chemical reactions).
Heat-driven Wastewater Treatment (HDWWT)		These are a specific type of wastewater treatment technologies which use thermal energy as the driving force, with a relatively lesser input of electric energy; The treated water streams at the outlet of HDWWT units (having an associated near-zero concentration of contaminants) may then be recirculated; The installation of these technologies potentially highly promotes the effectiveness of water recirculation within a water system, owing to the high capacity of contaminant removal.
Energy recovery from water or Wastewater-to-energy (WWtE)		This type of technologies subsist not in the direct use of water and heat streams but rather on the use of the discharge streams from the water system (both the discharge water stream and the sludge streams which result as by-products in WWT units) [29]; These discharge streams may be furtherly valorised to produce additional quantities of fuels (for instance, biofuels and synfuels) which may be furtherly used in combustion-based processes (in addition to used primary fuel, such as natural gas) [85].
	Thermochemical Water Splitting	It consists in a set of thermochemical cycles whose overall material input is liquid water and overall output is gaseous hydrogen and oxygen [160]; The assessment for the implementation of this technology subsist on the analysis of the availability of water streams that result as an output from a plant, the availability of heat source and cost-related limitations [160]. Thermochemical cycles that are commonly used for the occurrence of thermochemical water splitting include metal oxide cycles, sulphur-iodine (S-I) cycles and iron-chloride (Fe-Cl) cycle.

Table 2-5. Characterization of HR Technologies and Strategies

Technology	Characterization	Ref.
	Heat Exchanging Units	
Air-gas heat exchangers (Air preheaters)	Commonly applied in the use of waste heat from exhaust gases originated in combustion processes to an air stream, having different configurations (recuperator, regenerator, rotary regenerator and run around coil units) and designs (plate heat exchangers and heat pipe heat exchangers);	[161–173]
Liquid-gas heat Exchangers (Economisers)	Applied for the heating of the liquid stream, such as a water stream at the inlet of a boiler or a steam boiler; Associated typical fuel savings of 5 - 10% and a typical payback time of less than 2 years.	[174–178]
Heat Recovery Steam Generators (HRSG)	Highly complex technologies commonly applied to generate steam to be used in process heating within a plant and within the operation of thermodynamic cycles in order to produce electric energy; These heat exchangers are normally constituted by an economiser (in which the liquid stream is preheated in order to attain the boiling point), an evaporator (in which the saturated liquid is converted into vapour) and a superheater (in which the vapour is overheated beyond its saturation point); Make possible to attain an overall plant efficiency of 85 - 90% and electricity generation system efficiency of 75 to 85%.	[179,180]
	Electricity Generation Thermodynamic Cycles	
Organic Rankine Cycle (ORC)	System similar to the Clausius-Rankine cycle (CRC) (the working principle of the ORC consists in the capture of thermal energy from a heat source to evaporate an organic fluid), implemented for low-grade WHR; It is generally constituted by a turbine, a HRSG unit, a condenser and a pump (in many installations a regenerator is also installed to even further increase the system efficiency); The selection of the appropriate working fluid may lead to about 6 % increase of overall plant efficiency: the organic fluids R-12, R-123, R134a, and R-717 have been demonstrated as suitable to produce high efficiency systems and considerable production of electric energy; It has an associated payback time of 4 – 5 years.	[181–188]
Kalina Cycle	System similar to the CRC and ORC using water-ammonia mixture as the working fluid, suitable for medium and high temperature applications; Structurally similar to the Regenerative ORC although it is constituted by an additional separator due to the high ammonia concentration of the turbine outlet gas stream (so to assist on the full condensation of the water-ammonia mixture); It has an overall better WHR performance compared to the ORC, although the ORC requires less maintenance;	[189–193]
Supercritical CO_2 Brayton Cycle (SCBC)	System which has a similar arrangement to a common Brayton cycle and uses CO_2 at supercritical state as the working fluid; It has several advantages relative to other thermodynamic cycles, such as higher thermal efficiency, the opportunity to operate at a lower pressure across the system and the reduction of number of stages in the turbine; The heat extraction capability may be limited due to the heat transfer in the heater being processed in a low temperature range close to the maximum cycle temperature.	[194–196]

Table 2-6. Characterization of TES Technologies and Strategies

Technology	Description	Ref.
Liquid Thermal Tank	It is a sensible TES technology based on the heating of a liquid continuum within a tank; According to operational requirements, a liquid thermal tank may have several configurations, with different material streams being used as heat source streams, in addition to solar thermal collectors and a boiler unit, with a type of configuration being presented in Figure 2.6 – a); Liquids used for this type of STES component include, in addition to water (working temperature of 0 – 100 ºC), thermal oils (working temperature of 0 – 400 ºC), molten salts (working temperature of 150 – 565 ºC) and sodium (working temperature of 100 – 882 ºC).	[86,197–200]
Phase change material (PCM) Buffer	It is a latent TES technology based on the heating of a phase change material (PCM) continuum within a buffer, as represented in Figure 2.6 – b); The PCM buffer component is commonly part of water systems in which the water stream is heated up through the transportation in coils in its turn heated up by solar thermal collectors and then being transported to the buffer, as may be observed in Figure 2.7 – a); The type of systems aforementioned may be also coupled with a water thermal tank for improved overall performance of the TES system; Organic PCM's commonly used for this type of systems (or rather DHW systems that may be upscaled to process industry plant cases) include: paraffin wax, stearic acid, sodium acetate, lauric acid, myristic acid, palmitic acid and polyethylene glycol 6000; Inorganic PCM's used for this type of systems include: several salt hydrates, sodium carbonate and RT42-graphite.	[27,201–235]
Phase change material (PCM) heat exchanger	It is a latent TES technology consisting in a heat exchanger operating in a dynamic mode; A specific application of this technology includes the preheating of combustion air at the inlet of a combustion-based process using an exhaust gas stream as the heat source, as may be observed in Figure 2.7 – b); In the aforementioned system, the transportation of the exhaust gas stream to the PCM-TES unit works as the charging phase (in which the PCM phase in its turn is almost completely melted) and the transportation of the air stream works as the discharging phase (in which the PCM phase in its turn is again solidified by releasing the latent heat); Commonly applied material for the design of PCM-based heat exchangers include molten salts, metal alloys and eutectic inorganic PCM's.	

Table 2-7. Characterization of Thermochemical Energy Storage Technologies

Technology	Description	Ref.
Adsorption heat storage (AHS)	It is based on the phenomena of desorption (charging) and adsorption (discharging) of an air stream; Adsorption materials include zeolites (for desorption temperatures up to 180 ºC and adsorption temperatures up to 80 ºC), aluminophosphates/ silico-aluminophosphates (for desorption temperatures of 95 – 140 ºC and adsorption temperatures of 30 – 40 ºC) and metal organic frameworks (for desorption temperatures of 90 – 140 ºC and adsorption temperatures of 30 – 40 ºC); The configurations for AHS may be classified into open and closed systems, as may be observed in Figure 2.8.	[236–241]
Ammonia-based energy storage	It is based on the reactions of dissociation/ synthesis of ammonia (NH_3) into/ from nitrogen gas (N_2) and hydrogen gas (H_2); While the dissociation reaction is endothermic and corresponds to the charging phase, the synthesis reaction is exothermic and corresponds to the discharging phase; It is overall associated to the following advantages: • The reaction is single-step and does not require careful control; • The reactants and products are stable at operating temperatures; • The reactants and products are relatively abundant; • Possibility for the storage of liquid phase (NH_3) and gas phase (N_2 and H_2) within the same tank due to density differences; Operating temperatures overall vary within the range 400 – 1000 ºC; The industrial system typically includes two reaction vessels (for dissociation and synthesis), a separation and storage tank and two heat exchangers, as represented in Figure 2.9 – a). **Reactions** Haber–Bosch synthesis (Endothermic) $\mathrm{NH_3 \rightarrow \frac{1}{2}N_2 + \frac{3}{2}H_2,\ \Delta H^0 = 91.8\ kJ/mol}$ (CE1)	[242–248]
Calcium-looping energy storage	It is based on the reactions of calcination/ carbonation of calcium carbonate ($CaCO_3$) into/ from calcium oxide (CaO) and carbon dioxide (CO_2); While the calcination reaction is endothermic and corresponds to the charging phase, the carbonation reaction is exothermic and corresponds to the discharging phase; While carbonation occurs at about 650 ºC, calcination occurs in much higher temperatures; The industrial system encompasses three vessels for carbonate, calcium oxide and carbon dioxide, as represented in Figure 2.9 – b). **Reactions** Calcination (Endothermic) $\mathrm{CaCO_3 \rightarrow CaO + CO_2,\ \Delta H^0 = 160 - 172\ kJ/mol}$ (CE2)	[249–253]
Metal oxide energy storage	It is based on the reactions of oxidation/ reduction of metal oxides; The oxidation reaction is endothermic and thus corresponds to the charging phase, while the inverse reduction reaction is exothermic and corresponds to the discharging phase; The operational temperatures for the occurrence of reaction are set in the range of 700 – 1400 ºC; A typical industrial installation includes the supply of a heat source for the occurrence of reduction reaction and a reactor for the occurrence of the oxidation reaction, as represented in Figure 2.9 – c). **Reactions** Reduction (Endothermic) $\mathrm{MO_n \rightarrow MO_{n-\delta} + \frac{\delta}{2}O_2}$ (CE3)	[254–259]

Table 2-8. Characterization of HDWWT Technologies

Technology	Characterization		Ref.
Multi-effect distillation (MED)	It is a HDWWT technology associated to several operational advantages such as: • Use of low temperature operational levels; • Production of high quality treated water; • High thermal performance, use of low pumping power; • Requirement of minimum water pre-treatment; • Requirement for minimum labour.	It has limitations at the level of • Investment (highly expensive technology); • Considerable susceptibility to corrosion; • Existence of relatively low recovery ratio.	[11,260–265]
	A conventional MED unit may be divided into three sections: • The first effect section (in which the heat source is a hot liquid); • The second-to-last effects section (in which the heat source is the vapour stream produced in the immediately previous effect for each particular effect); • The condenser section (which condensates the last effect outlet vapour stream through heat transfer with the cold inlet saline water stream); The overall process at a conventional MED unit (schematically summarized in Figure 2.10 – a)) occurs as following: • The inlet saline water stream is distributed onto the first effect heat exchanger surfaces (being heated by a sensible heat source), producing a vapour stream; • The vapor stream then condenses in the next-effect heat exchanger and it serves a heat source for the feed water stream that is distributed in the same effect; • Also, within the second effect, the brine (concentrate) is purged; • Such process occurs until the last effect; • From the last effect, the corresponding vapor stream is transported to a condenser section, being condensed by the incoming saline water acting as a coolant; Being considered a distillation process, it is set to remove the following water contaminants in addition to dissolved salts: organic compounds, heavy metals (such as lead), chlorine, chloramines, radionuclides and microorganisms, but potentially fails in the removal of contaminants that are more volatile than water (such as determinate pesticides, volatile solvents, and volatile organic compounds).		
Multi-stage flash distillation (MSFD)	It is a HDWWT technology with an operation principal similar to MED, being associated to the advantage of having a higher resistance against scaling compared to MED, in addition to: • Large capacity for freshwater production; • Independence from the salinity of feed water; • Operation and maintenance simplicity; • Low performance degradation; • Production of high quality freshwater; • Potential for combination to other processes;	It is associated to disadvantages at the level of: • Investment (high investment technology); • Requirement for high level technical knowledge; • Highly thermal energy intensive process (high operational temperatures); • Low recovery ratio;	[260,264–271]

	The overall process of MSFD occurs (schematically summarized in Figure 2.10 – b)) occurs as following: • The feed water stream is discharged into a series of flashing chambers (at an operation pressure slightly below than the saturation vapour pressure), being pressurized and heated up with a fraction of the feed water stream being vapourised; • The vapourised fraction of the feed water stream is then transported through a mist eliminator and it is condensed at the exterior surface of a condenser located at the top of each stage of the MSFD; • The condensed treated water stream is then dripped into trays and collected; Being considered a distillation process, it is set to remove the following water contaminants in addition to dissolved salts: organic compounds, heavy metals (such as lead), chlorine, chloramines, radionuclides and microorganisms, but potentially fails in the removal of contaminants that are more volatile than water (such as determinate pesticides, volatile solvents, and volatile organic compounds).	
Membrane distillation (MD)	It is a heat-driven membrane technology associated to several advantages in relation to conventional distillation technologies such as: • Low energy requirements; • Non-dependability from concentration polarization; • Lack of limit in feed water concentration; It is associated to disadvantages at the level of: • Investment cost (high investment cost associated to MD module); • Possibility of membrane wetting in the case of the presence of surfactant and amphiphilic contaminants; The overall operation of a MD module occurs as following: • Initially, at least one side of the microporous hydrophobic membrane is in direct contact with wastewater; • The temperature gradient between the two sides of the membrane induces partial pressure difference, which in its turn is the driving force for mass transfer through membrane pores and evaporation of volatile compounds; • The vapourised fraction is then condensed on the permeate side of the membrane; The temperature gradient within the MD module may be generated by the implementation of a heat recovery system which may be: • Single-loop as represented in Figure 2.10 – c) (the heat source is directly connected to the membrane); • Two-loop as represented in Figure 2.10– d) (in which a heat exchanger is implemented, and also commonly a TES unit for time-dependent systems); The MD module may have several configuration: • Direct contact membrane distillation (DCMD); • Vacuum membrane distillation (VMD); • Air gap membrane distillation (AGMD); • Sweeping gas membrane distillation (SGMD); Being considered a distillation process, it is set to remove the following water contaminants in addition to dissolved salts: organic compounds, heavy metals (such as lead), chlorine, chloramines, radionuclides and microorganisms, but potentially fails in the removal of contaminants that are more volatile than water (such as determinate pesticides, volatile solvents, and volatile organic compounds).	[264,265,272–276]

Table 2-9. Characterization of WWtE Technologies

Technology	Description	Ref.
Anaerobic Digestion	• It is a process in which the output is primarily biogas, with a digestate resulting as the by-product; • It is prominently applied for the treatment of wastewater streams with a significant load of organic materials, which are considerable prone to biological degradation; • The produced biogas may be injected in natural gas networks, through the process of separation of carbon dioxide and other contaminants to turn biogas into biomethane; • The by-product (digestate) may be furtherly applied in agriculture; The anaerobic digestion process may be integrated in the operation of a WWT unit as represented in Figure 2.11 – a).	[277–283]
Gasification	• It subsists on the partial oxidation of biodegradable material present in wastewater streams for the production of synthesis gas (syngas), as well as a solid fraction of char as by-product; • The produced syngas is commonly composed by hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2) and methane (CH_4); • The produced syngas is an intermediate in the production of other fuel gases, such as diesel fuel (by Fischer-Tropch process) and hydrogen (which must be refined for its use in fuel cells); The gasification process may be integrated in the operation of a WWT unit as represented in Figure 2.11 – b).	[284–289]
Electrolysis	• It is a process that uses an electric current to produce hydrogen, based on oxidation-reduction reactions; • A set of by-products (such as chlorine and sodium hydroxide) may also be generated, as represented in Figure 2.11 – c); • Several types of electrolysis processes exist, such as: alkaline water electrolysis, solid oxide electrolysis, microbial electrolysis and PEM water electrolysis; The produced hydrogen may be directly injected into the natural gas fuel supply to combustion-based processes, through processes of production of hydrogen-enriched natural gas (HENG).	[72,290–298]

Table 2-10. Characterization of Thermochemical Water Splitting (TWS) Technologies

<table>
<tr><th>Technology</th><th colspan="3">Description</th><th>Ref.</th></tr>
<tr><td rowspan="4">Metal oxide cycle</td><td colspan="3">It is a two-step thermal cycle based on the redox reactions of metal oxides, in which the reduction step (CE4) is endothermic and the oxidation step (CE5) is exothermic;
It presents the following advantages in comparison to the remaining thermal cycles:
• In terms of input-output streams, wastewater and heat are the only inputs and hydrogen and oxygen are the only outputs;
• The produced H_2 and O_2 are separated in different reactions;
• The existence of continuous recycling of reactants and products;
• The produced H_2 gas is pure.
Typical metal oxides implemented for this type of thermal cycle are: CdO/ Cd, ZnO/ Zn, SnO_2/ SnO, Mn_2O_3/ MnO, CeO_2/ Ce_2O_3 and Fe_3O_4/ FeO;
The operational temperatures across the cycle are in the range of 900 – 2000 ºC;
A typical installation encompassing this thermal cycle is represented in Figure 2.12 – a).</td><td rowspan="4">[299–315]</td></tr>
<tr><td colspan="3">Reactions</td></tr>
<tr><td>Reduction</td><td>$\mathrm{MO_n \rightarrow MO_{n-\delta} + \frac{\delta}{2} O_2}$</td><td>(CE4)</td></tr>
<tr><td>Oxidation</td><td>$\mathrm{MO_{n-\delta} + \delta H_2O \rightarrow MO_n + \delta H_2}$</td><td>(CE5)</td></tr>
<tr><td rowspan="5">Sulphur-iodine cycle</td><td colspan="3">It is three-step thermal cycle based on the use of sulphur and iodine components, in which the sulphuric acid decomposition (CE6) and Bunsen reaction (CE7) are endothermic and iodic acid decomposition (CE8) is exothermic;
It has the advantage of being a significantly high efficiency hydrogen production system, although it as an associated drawback of the involvement of high corrosive sulphuric and iodic acids (which requires, for instance, a higher attention on security);
In terms of operational temperatures, the sulphuric acid decomposition typically occurs at about 120 ºC, the Bunsen reaction above 800 ºC and the iodic acid decomposition above 350 ºC;
A typical installation of this thermal cycle is represented in Figure 2.12 – b).</td><td rowspan="5">[316–319]</td></tr>
<tr><td colspan="3">Reactions</td></tr>
<tr><td>Sulphuric acid decomposition</td><td>$\mathrm{H_2SO_4 \rightarrow SO_2 + H_2O + {}^1/_2\, O_2, \Delta H^0 = +186\ kJ/mol}$</td><td>(CE6)</td></tr>
<tr><td>Bunsen reaction</td><td>$\mathrm{I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4, \Delta H^0 = -75\ kJ/mol}$</td><td>(CE7)</td></tr>
<tr><td>Iodic acid decomposition</td><td>$\mathrm{2HI \rightarrow I_2 + H_2, \Delta H^0 = +12\ kJ/mol}$</td><td>(CE8)</td></tr>
<tr><td rowspan="6">Iron-chlorine cycle</td><td colspan="3">It is a four-step thermal cycle based on the use of iron and chlorine components, in which the reverse Deacon reaction (CE9) and hydrolysis (CE10) are endothermic and thermal decomposition (CE11) and chlorination (CE12) are exothermic;
In terms of operational temperatures, thermal decomposition occurs at 425 ºC, the reverse Deacon reaction and hydrolysis in the range 525 – 925 ºC and chlorination at 125 ºC;
A typical installation of this thermal cycle is represented in Figure 2.12 – c).</td><td rowspan="6">[320–322]</td></tr>
<tr><td colspan="3">Reactions</td></tr>
<tr><td>Thermal Decomposition</td><td>$\mathrm{2FeCl_3 \rightarrow 2FeCl_2 + Cl, \Delta H^0 = -160.5\ kJ/mol}$</td><td>(CE9)</td></tr>
<tr><td>Reverse Deacon Reaction</td><td>$\mathrm{Cl_2 + H_2O \rightarrow 2HCl + {}^1/_2\, O_2, \Delta H^0 = +59.4\ kJ/mol}$</td><td>(CE10)</td></tr>
<tr><td>Chlorination</td><td>$\mathrm{Fe_3O_4 + 8HCl \rightarrow FeCl_2 + 2FeCl_3 + 4H_2O, \Delta H^0 = -244\ kJ/mol}$</td><td>(CE11)</td></tr>
<tr><td>Hydrolysis</td><td>$\mathrm{3FeCl_2 + 4H_2O \rightarrow Fe_3O_4 + 6HCl + H_2, \Delta H^0 = +156\ kJ/mol}$</td><td>(CE12)</td></tr>
</table>

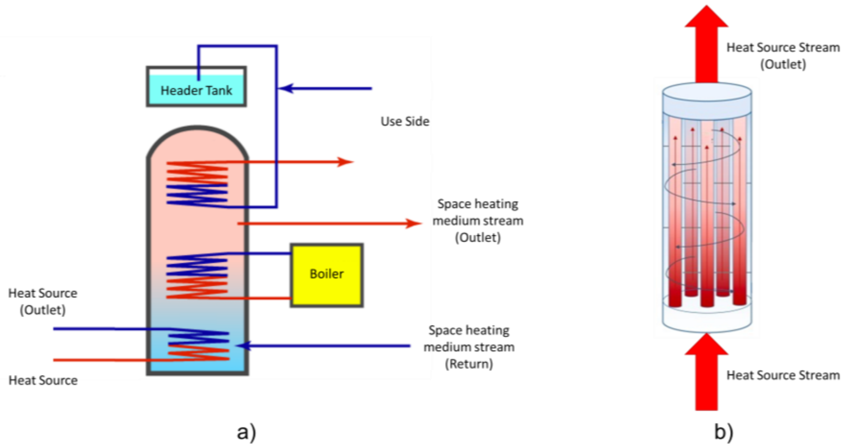


Figure 2.6. Representations of TES Technologies: a) Water thermal tank, b) Generic phase change material (PCM) unit considering the inlet and outlet of the heat transfer fluid (adapted from [200] and [323])

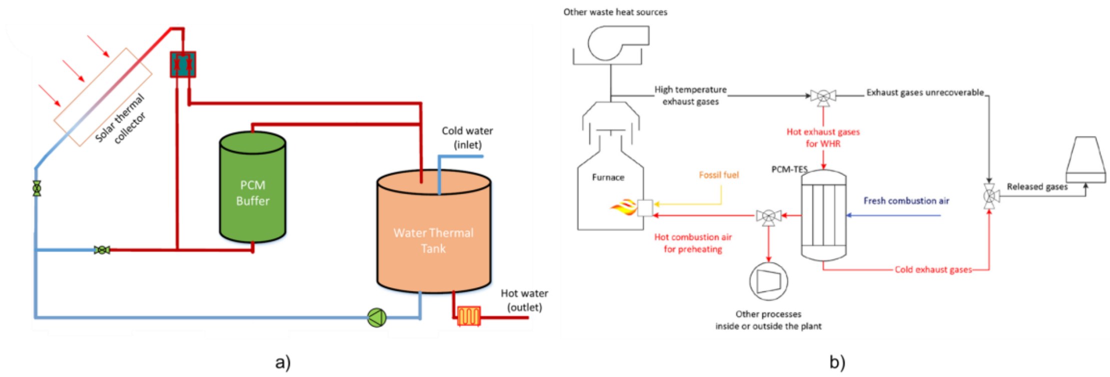


Figure 2.7. Flowsheet of: a) Sensible and latent energy storage system integrated in a water circuit, b) Application of a PCM-based heat exchanger for air preheating (adapted from [27] and [212])

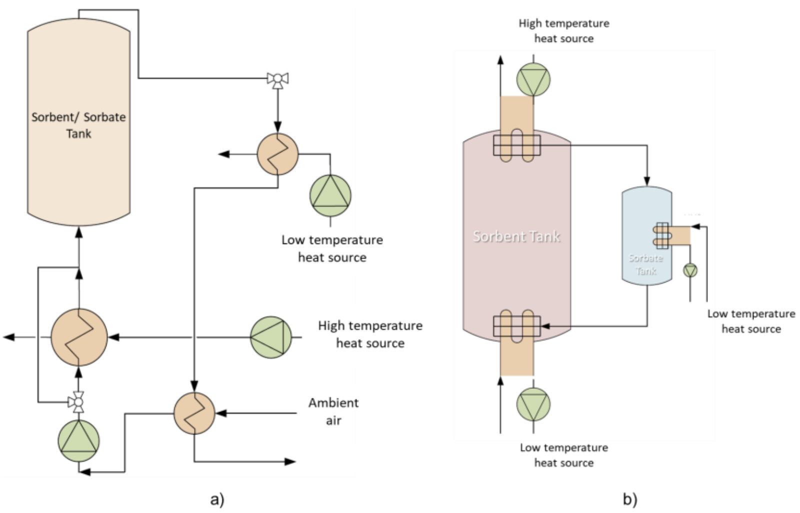


Figure 2.8. Flowsheet for a) Open adsorption heat storage system, b) Closed adsorption system (adapted from [239])

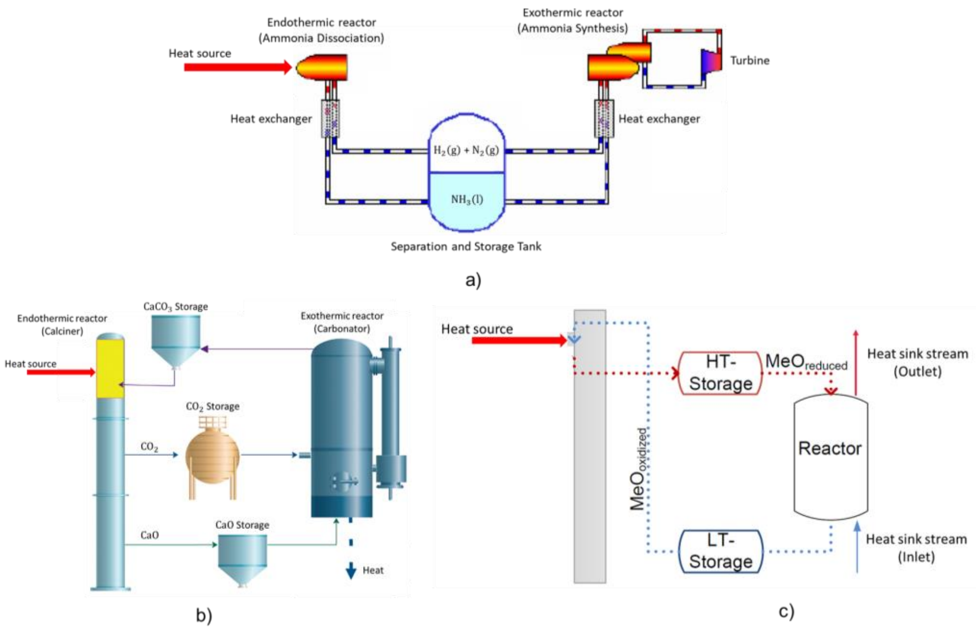


Figure 2.9. Flowsheet for a) Ammonia-based energy storage, b) Calcium-looping energy storage, c) Metal oxide cycle-based energy storage (adapted from [248] and [252])

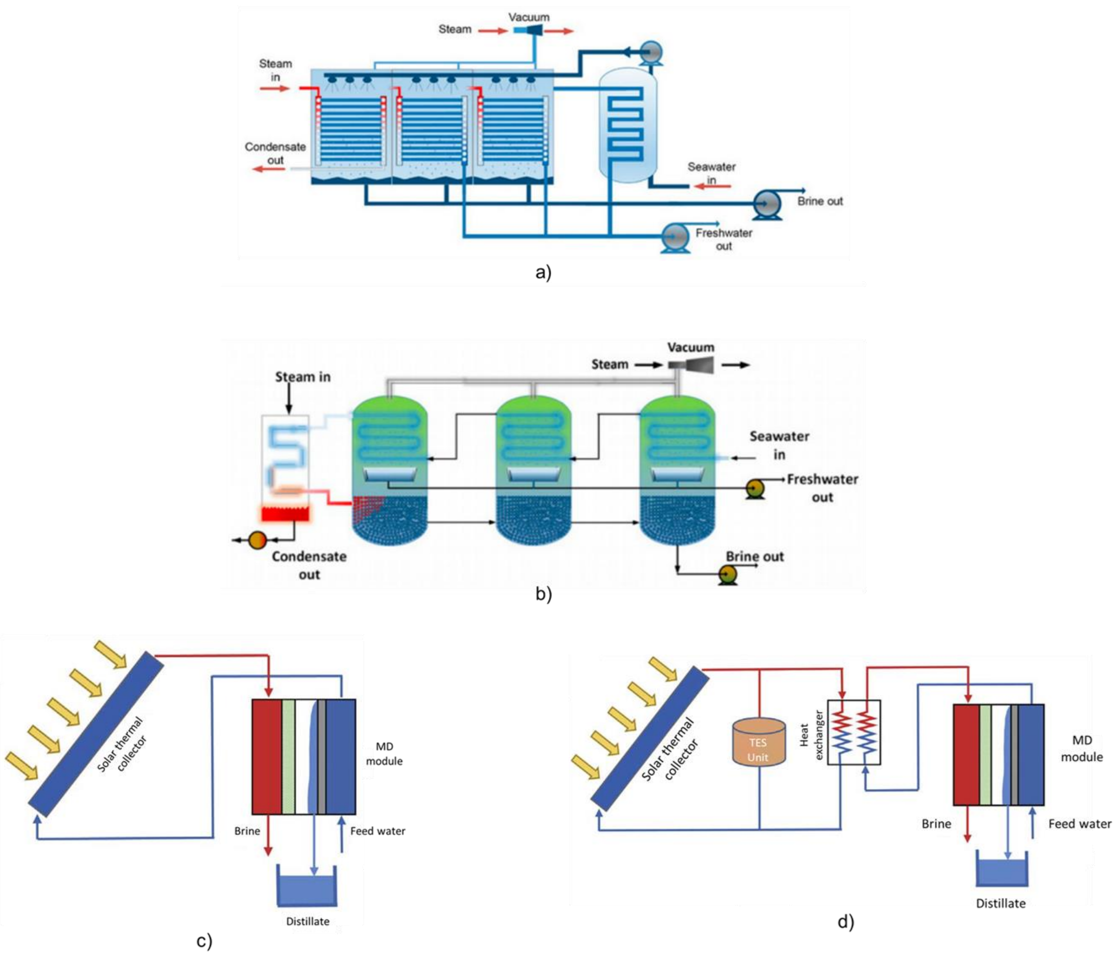


Figure 2.10. Flowsheet representations for Heat-driven WWT technologies: a) Multi-effect distillation (MED), b) Multi-stage flash distillation (MSFD), c) single-loop Membrane Distillation (MD), d) two-loop Membrane Distillation (MD) (adapted from [271] and [272])

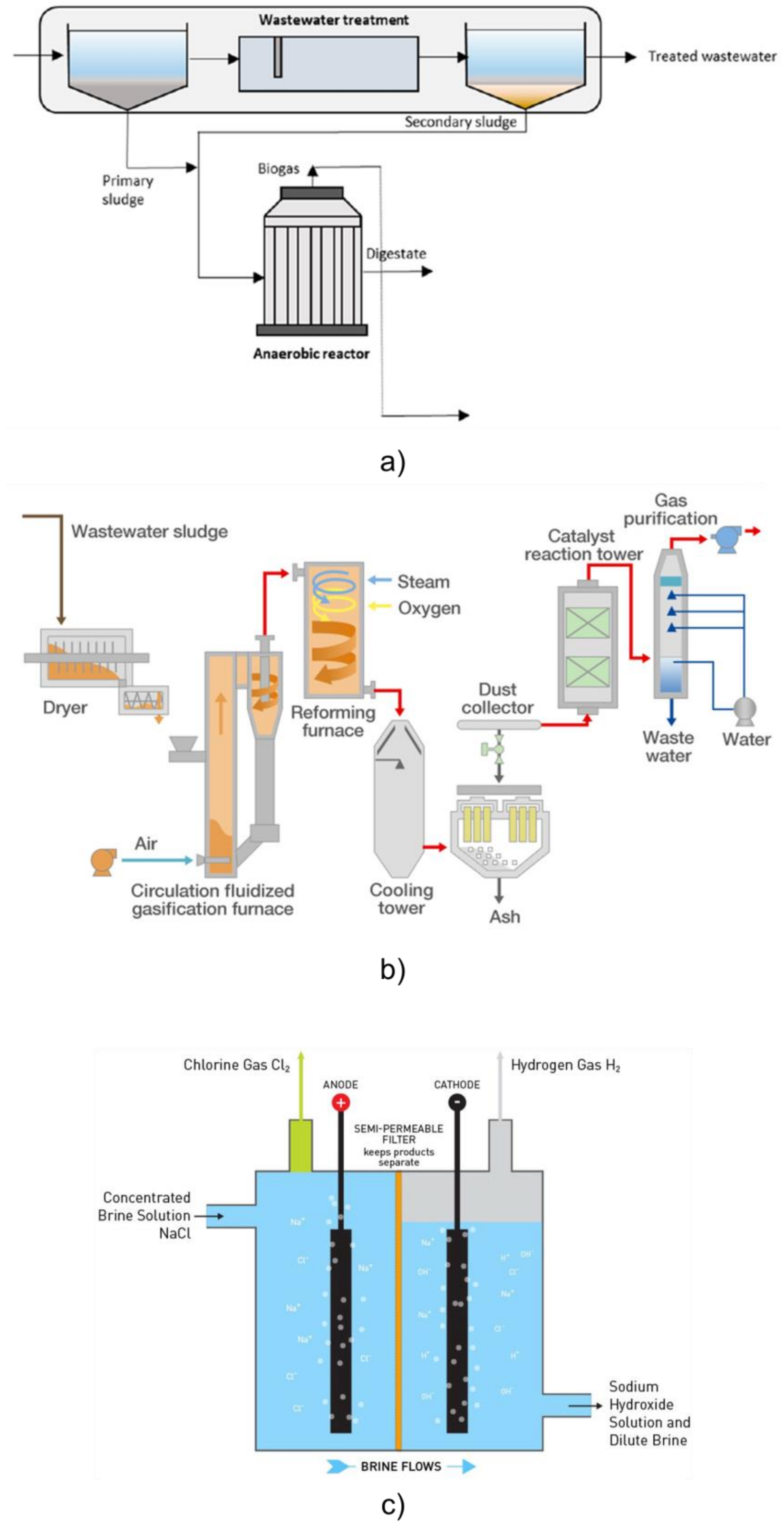


Figure 2.11. Flowsheet representations for WWtE technologies: a) Anaerobic Digestion, b) Gasification, c) Electrolysis (adapted from [277], [288] and [291])

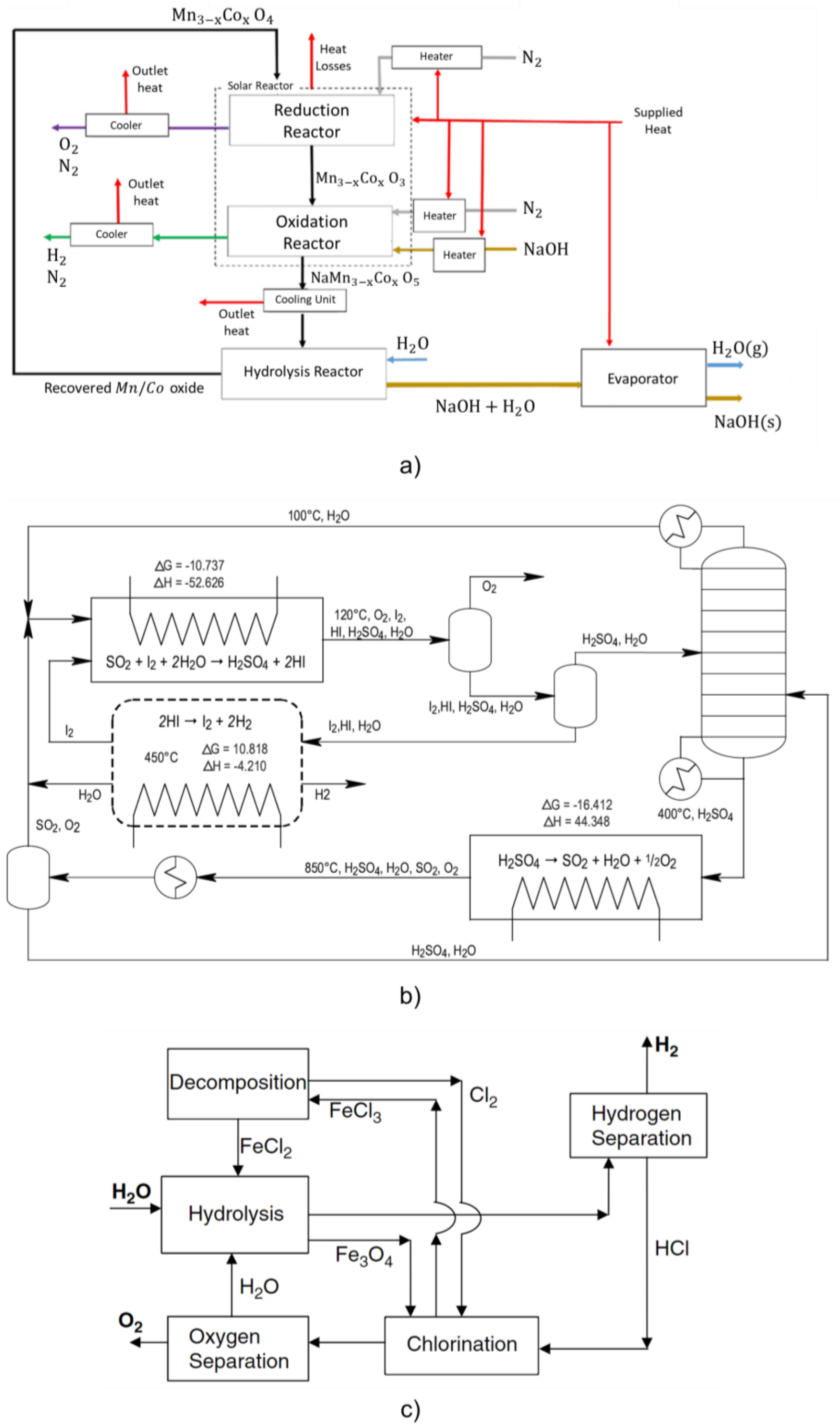


Figure 2.12. Flowsheet representations for thermochemical water splitting systems: a) Metal oxide cycle, b) Sulphur-iodine cycle, c) Iron-chlorine cycle (adapted from [307], [319] and [322])

2.5. Model Development and Computational Methods

The numerical modelling work required for the ultimate objective of the conceptualization of energy recovery and water recirculation systems subsists on the exploitation of several industrial equipment components and physical phenomena. The equations necessary to gather in order to develop a model of an industrial system may be summarized to the equations that describe the phenomena occurring within a determinate component (such as heat transfer, mass transfer, energy storage and chemical reactions) and the flow of material and energy streams between several industrial processes. In general, the models set to be conceptualized for this work may be classified into two types:

- **Simulation models** (models with zero degrees of freedom), which are set to be developed for the analysis of the occurring phenomena and the determination of several indicators related to the energy and environmental performance of the industrial system, with the overall system models essentially consisting on the assembling of the flowsheet of the aforementioned plant section;
- **Optimisation models** (models with more-than-zero degrees of freedom), which are set to be developed for the assessment of optimal points of the operation of the system in which the recirculation of water and heat source streams generates the maximum possible eco-efficiency (although the objective-functions required to be enunciated may consist on the minimization of water, energy and investment-related costs).

Moreover, each one of the aforementioned may be classified into:

- **Steady state models**, in which it is verifiable the inexistence of appreciable variations of the variables and equations describing the occurring phenomena with time;
- **Dynamic models**, in which the occurring phenomena is analysed and assessed based on the obtainment of graphs for time-dependent variables and whose enunciated equations include time-dependent variables).

The conceptualization of energy recovery and water recirculation systems is set to be analysed by the means of the assessment of the optimal point of the operation of the overall system, which basically consists of the point in which the water and energy consumption are the least possible while respecting all the operational constraints. At the light of computational works, such assessment may be performed by the application of optimisation methodologies. All the optimisation models, in this case, must be developed considering the objective-function of the reduction of the total investment cost associated to the effective implementation of energy recovery and water recirculation systems, which encompasses not only the costs associated to water and energy use but also the costs associated to the acquisition of technologies, as well as other investment costs parcels such as the ones related to maintenance.

In Table 2-11, it is performed a synthesis of all the optimisation methods applicable for heat recovery systems and water-energy networks.

Table 2-11. Synthesis of computational methods applied for Heat Recovery Systems and Water Networks

Method	Characterization	Method
	Heat Recovery Systems	
Linear and Non-linear Programming	It is based on the application of standard optimisation methods in which the governing equations of industrial systems are formulated as equality constraints and the objective functions are set as the summation of capital costs (associated to the system implementation) and operating costs (associated to water and energy use); Under determinate circumstances, the models may be adapted so that non-linear equality constraints are linearized.	[324–331]
Multi-objective Programming (MOP)	It is based on the attainment of the minimization of several indicators related to energy use and equipment sizing; It is commonly based on bi-objective problems, in which the Pareto set encompasses two of these variables: energy efficiencies, exergy efficiency energy consumption levels, investment costs and equipment-related areas; It is commonly implemented for the optimisation related to ORC encompassing systems; A potential disadvantage is the issue of rank reversal associated to the use of TOPSIS procedures.	[332–335]
Dynamic Programming (DP)	It is applicable for heat recovery systems with time-dependent variables, such as the ones containing TES units; The objective function is formulated (in a general form) as the minimization of supplied thermal power during a determinate time period (defined as an integral).	[336–340]
Graphical Methods	It is based on the application of the pinch analysis methodology for the planning of heat exchanger networks (HEN); The application of graphical methods may be concomitantly use for equipment design purposes, namely in respect to the calculation of heat transfer areas.	[341–345]
	Water-Energy Networks (WEN)	
Linear and Non-linear Programming	It is based on the application of standard linear and non-linear methods; It generally subsists on the planning of WEN superstructures, with the objective function being the summation of water and energy costs (which are generally linear) and heat exchanger-related costs (which are generally non-linear); It has limitations in the finding of optimal solutions, as in general only local optimal solutions are attained.	[190,192,193, 197,198,201, 203–208,210, 212,302,303]
Multi-objective Programming (MOP)	It is based on the minimization of pairs of variables associated to the WEN, namely water costs, utilities costs and heat exchanger units; It has associated limitations in terms of the handling of the genetic algorithms with equality constraints (such as mass and enthalpy balance equations that must be necessarily enunciated within the model).	[96,347]
Graphical Methods	The two types of graphical-based approaches are applied for WEN conceptualization: Combined application of water pinch analysis and heat pinch analysis methodologies; P-graph framework (based on the mapping of all operating units and potential material flows).	[84,85,194, 196,199,202]

Within the scope of water and energy integration, the existing and commonly used optimisation methods are essentially of two types: the pinch analysis method (which is a graphical method) and mathematical programming (MP):

- The pinch analysis method is associated to several benefits, such as being based on a holistic perspective for the application of a systematic approach for the planning of industrial systems, although it majorly suffers from drawbacks at the level of simulation performance (it is a method conceptualized in a steady-state perspective) and at the level of modelling (simple models of the whole systems considering a high number of assumptions on fluid properties and temperature profiles) [348];
- In the scope of this work, the application of mathematical programming methods will be favoured over the use of graphical methods such as pinch analysis. Mathematical programming relevantly includes methods such as linear and non-linear programming (which is a set of methods which includes LP, NLP, MILP and MINLP), multi-objective programming (MOP) and dynamic programming (DP).

As may be evidenced in Table 2-11, the research on the optimisation of water-energy networks (WEN) is at the date a much more profoundly developed area in comparison to heat recovery systems. The field of the optimisation of WEN has associated the development and implementation of several proper state-of-the-art models and algorithms, while for heat recovery systems the applied methods are summarized to the standard optimisation methodologies. Nonetheless, it is to note that, while for WEN the set-to-be conceptualized superstructures include only the water-using processes, WWT units and heat exchangers, the conceptualization of heat recovery systems requires the analysis and assessment of the implementation of a higher number of existing technologies, which in this prospect reflects the lack of literature studies on optimisation methodologies subsisting on the implementation of one or more of these technologies in a planned manner.

In a further analysis, it is possible to verify the lack of the existence of dynamic programming studies for WEN. Such lack of studies may be simply attributed to the fact that the operational conditions associated to industrial processes encompassed in WEN do not appreciably vary during a determinate time period given for analysis, thus not requiring to analyse the minimization of a water and energy cost function for different successive time intervals. Attending to the requirement of the coupling of both these types of systems for the conceptualization of simultaneous heat recovery and water recirculation systems, it is to note that it is necessary to assess the most adequate form to frame the simultaneous application of a DP model for the sole case of a thermal process system and the steady state-based optimisation of a WEN. Since these two systems constituting a WEIS may be set to be relatively independent, in the sense that the enthalpy to be allocated from the thermal process system to the WEN (namely to the heaters and the heat-driven WWT units) may be set to be constant for a determinate time period, thus securing that only the thermal process system is the only required to be optimised in a dynamic perspective.

2.6. Sustainability Assessment Indicators

The assessment of the viability associated to the implementation of energy recovery and water recirculation systems primarily subsists on the analysis of the benefits potentially to be obtained, namely energy savings, water savings, GHG emission reduction and wastewater pollutant reduction. These benefits may be all translated to economic-based values by the means of monetary-based unitary factors (such as water and energy unitary costs and the costs associated to pollutant emissions). Nonetheless, a set of key performance indicators (KPI) may be defined. These KPI are set to subsist on the comparison of the implemented systems with:

- The formerly implemented case within the plant (the initial linear economy-based situation);
- Other systems (conceptualized and implemented for other case-studies).

Ultimately, these indicators are set to translate the promotion of eco-efficiency and circular economy character of an industrial system, by overall performing a customised energy and environmental performed assessment. In the perspective of plant operation improvement and the development of optimisation models for that end, the determination of these indicators is set to converge on potential gaps associated to decision-making by industrial and entrepreneurial stakeholders, namely in respect to operational conditions and plant-associated variables that are not accounted by the developed models. In Table 2-12, several KPI defined conceptualized for water and energy integration are presented.

Table 2-12. Characterization of key performance indicators applicable for energy recovery and water recirculation systems

Indicator	Units	Characterization	Ref.
		Water efficiency assessment	
Specific water consumption	m^3 Water/ ton material	It consists on the ratio between water consumption and the produced material in a process or the overall plant; It is commonly implemented in the prospect to assess the potential of several measures to reduce water use.	[349,350]
Economic value per dissipated water	€/ kg dissipated water	It consists of the ratio between the economic value associated to material production and the amount of dissipated water.	[351]
Wastewater Circonomics Index	None	It consists of an aggregated indicator that measures the circularity character of a water system. It is determined by the product of three sub-indicators: wastewater reuse indicator (measures the part of product mass relative to reusability), composite wastewater re-use indicator (a value-weighted indicator measuring the equivalent shadow prices of eliminated externalities) and wastewater recycle indicator (measures the ratio of the quantity of wastewater that is effectively used by economic activities). It is assessed an up to 50% water recirculation in process industry overall.	[352]
		Energy efficiency assessment	
Specific electric energy consumption	MWh_{el} /ton material	It is commonly used to assess the general energy efficiency associated to the overall use of electric energy in a process industry plant.	[353–356]
Specific thermal energy consumption	MWh_{th} /ton material	It is commonly used to assess overall energy efficiency associated to the fuel consumption on thermal processes.	
Produced material emission intensity	ton GHG/ ton material	It consists of the ratio between GHG emissions ($CO_{2_{eq}}$ and NO_X) and the produced material defined to an overall plant or a process; Considering that combustion-related emissions are highly superior to process emissions for all process industry thermal processes, it may be used to evaluate the emission intensity reduction potential associated to several measures.	[353,356]
Energy carbon footprint	ton $CO_{2_{eq}}$/ TJ	It consists of the ratio between equivalent CO_2 emissions and energy consumption (thermal and electric) in a plant in an overall perspective.	[357,358]
Thermal efficiency	None	It consists of the ratio between the useful thermal energy output and thermal energy input in a process industry thermal process.	[359]
		Aggregated	
Waste Heat Performance Ratio	kg water/ kg waste heat stream or GJ produced vapor/ GJ waste heat	It consists of the ratio between produced treated water and the used amount of a waste heat stream; On the context of heat-driven water treatment, it may be determined by comparing in terms of material quantities ratio between mass flow rate of produced treated water and waste heat stream) and energy quantities (ratio between produced vapour and supplied thermal energy).	[360,361]
Energy water footprint	m^3 Water/ TJ	It consists of the ratio of water consumption and energy consumption (thermal and electric) in a plant in an overall perspective.	[358,362]

2.7. Analysis of Water and Energy Use Levels in Portugal and the European Union

The existing methodologies for the solving of the concerns regarding the implementation of heat recovery and water recirculation systems are set to be applied in the context of several sectors of the overall process industry. While the existing methodologies are all-embracing in the aspect that the only aspect to take into account is the presence of water and energy-using units (rather than otherwise relevant characteristics of a plant of a specific sector), the attractiveness associated to the research on sustainability promotion in a determinate market pass by the analysis of the levels of water and energy consumption, as well as other economic and environmental-related indicators. In this sense, an industrial sector whose water and energy efficiency improvement studies may be classified as attractive is one whose levels of water use, energy use and GHG emissions have been identified as significant. The plants of each individual of these industrial sectors have all installed considerable quantities of combustion-based and water-using processes from which such methodological analysis is based on. This work is strategically framed within the markets of the European Union and (more specifically and in more detail) Portugal, and as such much of the overall study is adapted to the process industry reality of the referred region/ country.

2.7.1. Water and Energy Use Statistics

In Figures 2.13 – 2.16, several graphical representations of the water use, energy use and GHG emissions levels for Portugal and the European Union are presented. While Figures 2.13 – 2.15 subsist on average consumption levels (per number of enterprises in the region/ country), the respective absolute values are respectively represented in Figures A1 – A3 of the appendix A1. For the elaboration of the graphical representations presented in the sequence of Figures 2.13 – 2.16, numerical data present in available online databases and statistical analysis-based literature [21,363–366] have been conjointly gathered and used.

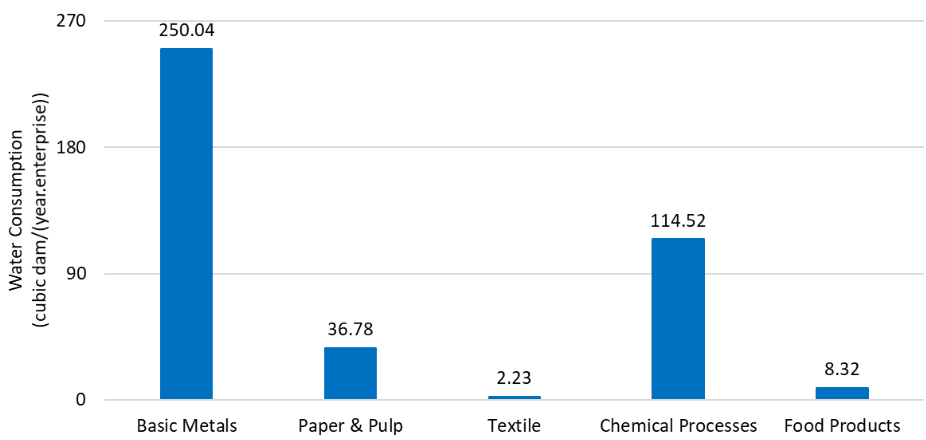


Figure 2.13. Estimated water consumption levels for several industrial sectors in the European Union (data gathered from [21,363–366])

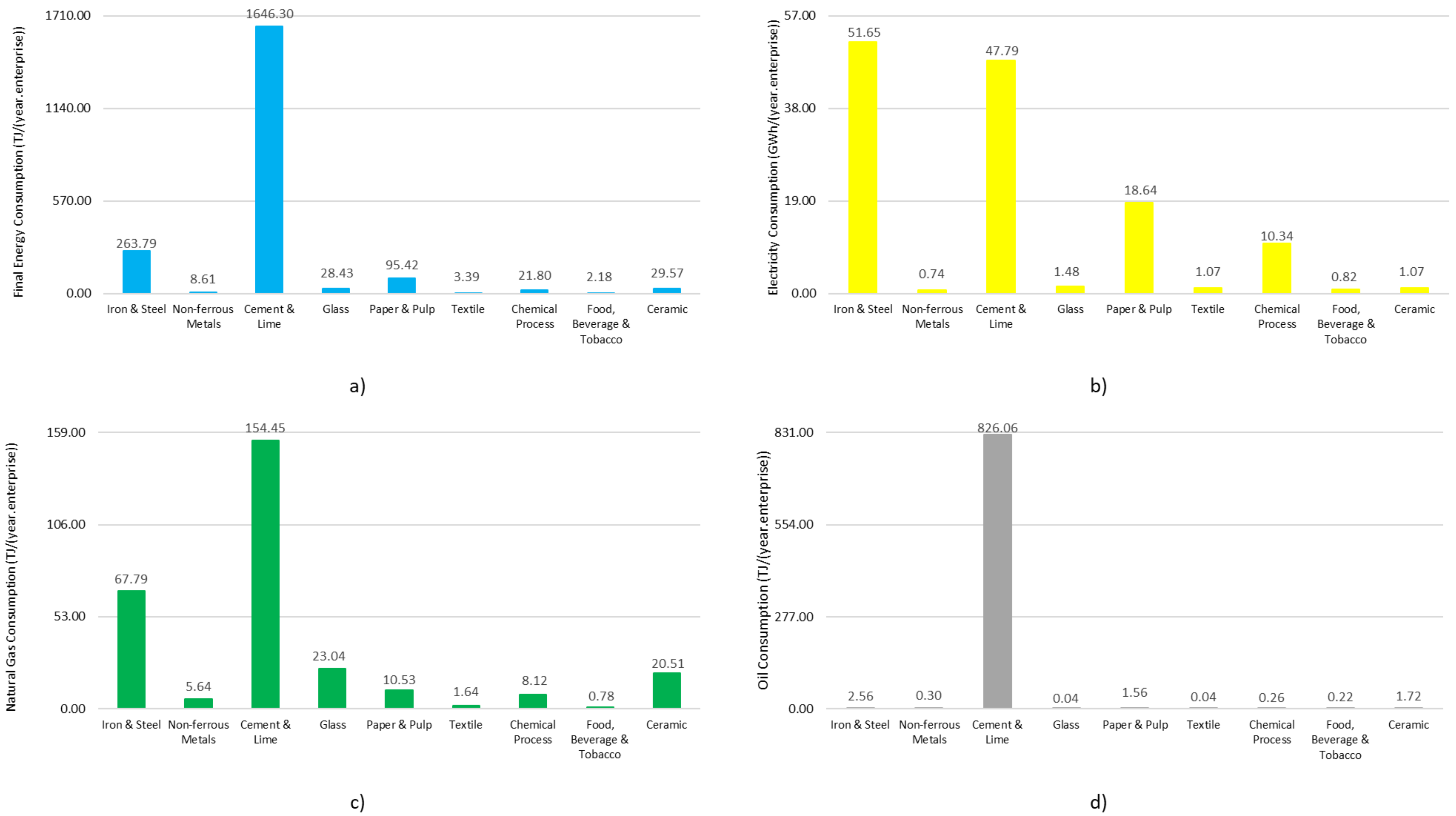


Figure 2.14. Final energy consumption levels per number of enterprises for nine process industry sectors in Portugal: a) Final Energy Consumption, b) Electricity Consumption, c) Natural Gas Consumption, d) Oil Consumption (reference years of 2020 for energy consumption levels and 2019 for number of enterprises) (data gathered from [21,363–366])

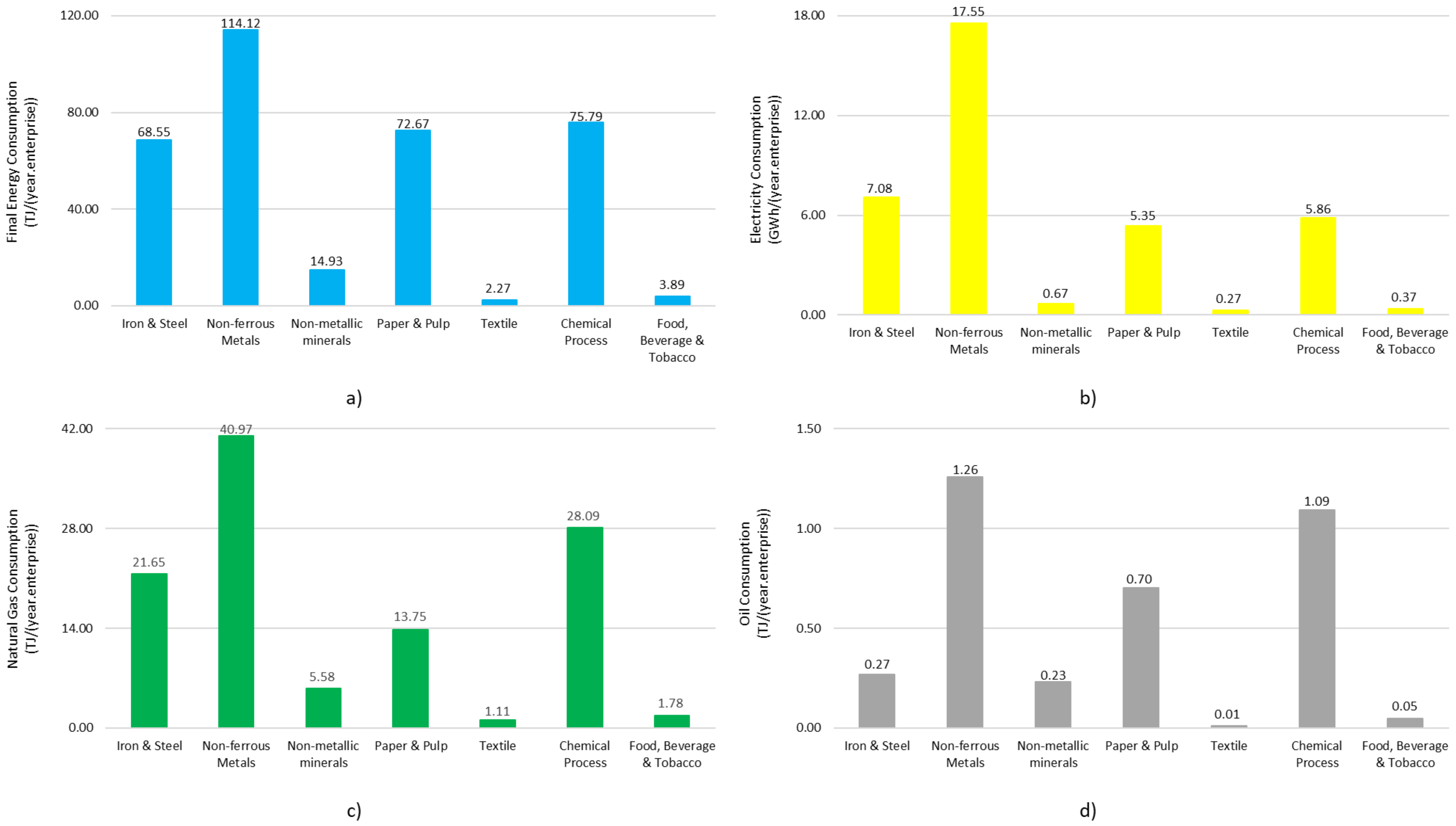


Figure 2.15. Final energy consumption levels per number of enterprises for seven process industry sectors in the European Union: a) Final Energy Consumption, b) Electricity Consumption, c) Natural Gas Consumption, d) Oil Consumption (reference years of 2021 for energy consumption levels and 2019 for number of enterprises) (data gathered from [21,363–366])

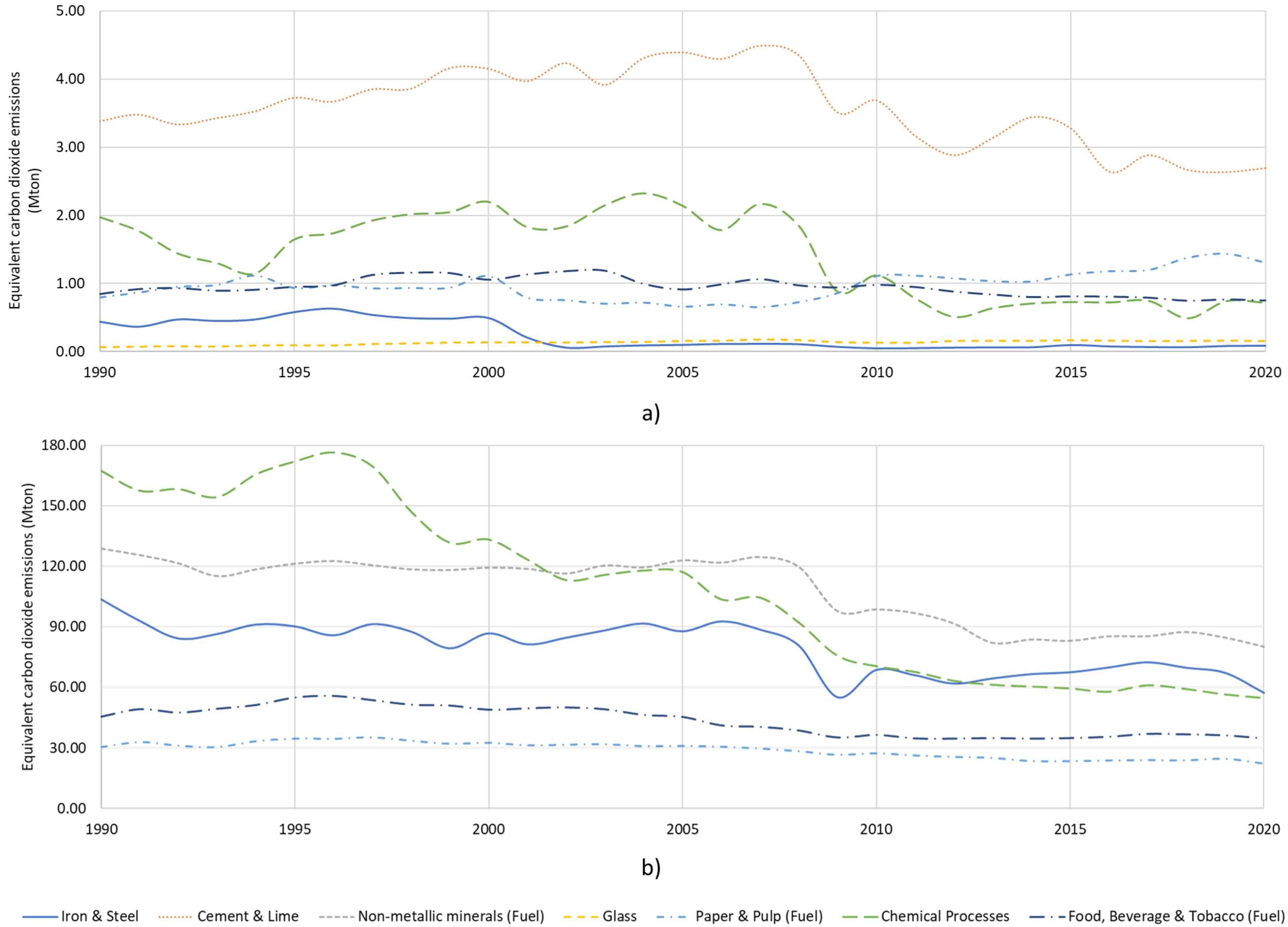


Figure 2.16. Equivalent carbon dioxide ($CO_{2,eq}$) emission levels for the 1990 – 2020 yearly period for several industrial sectors for a) Portugal and b) European Union (data gathered from [21,363–366])

2.7.2. Classification of Waste Heat Potential

The classification of waste heat potential is relevant in the way to attend to the water and energy efficiency improvement and decarbonisation requirements identified in the previous section. Such classification consists in categorising the waste heat streams existing in the plants of each process industry sector in typical temperature ranges and the corresponding measured waste heat potential. In Figure 2.17, the waste heat potential levels associated to several sectors in the context of the European Union are presented. In Figure 2.18, the waste heat potential measured in units of enthalpy (PJ/year) associated to defined temperature ranges is represented for each approached industrial sector. The categorisation of the waste heat potential in terms of the temperature range is performed in Table 2-13.

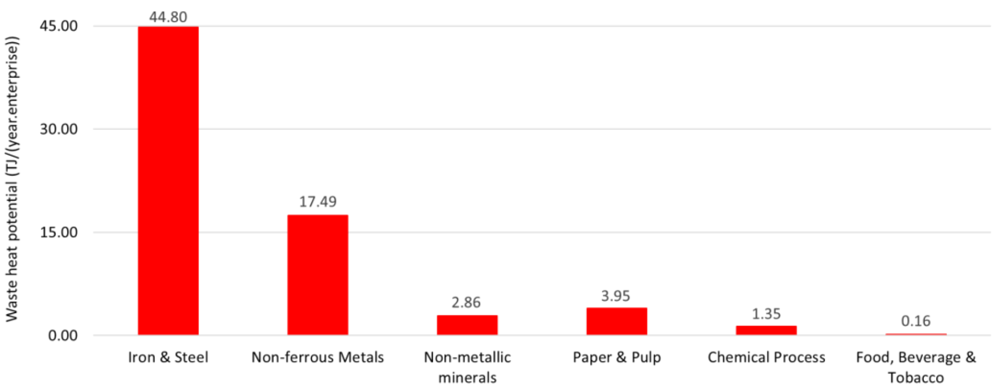


Figure 2.17. Waste heat potential levels for several industrial sectors in the European Union (data gathered from [21,363–366])

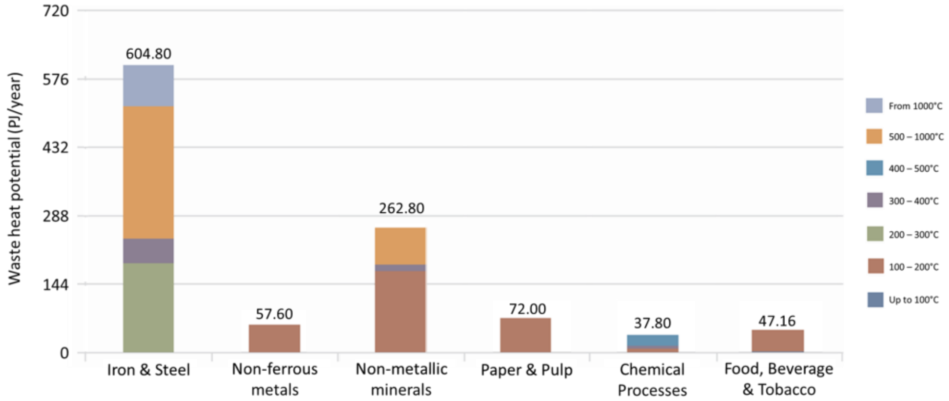


Figure 2.18. Waste heat potential levels for several industrial sectors in the EU (adapted from [363])

Table 2-13. Categorisation of waste heat potential according to temperature intervals

Category	Temperature Interval
Low	Up to 200 ºC
Medium	200 – 400 ºC
High	400 – 1000 ºC
Very high	From 1000 ºC

As may be observed by the analysis of Figure 2.18, the Iron & Steel sector is the one associated to the highest and most diverse (in terms of temperature ranges) waste heat potential, being the only one having waste heat streams in the category of very high potential. The Non-metallic minerals sectors have also a diverse set of temperature ranges, although the total waste heat potential is much lower than the one of Iron & Steel sector and the presence of low temperature waste heat streams are predominant. The Non-ferrous metals, Paper & pulp, Chemical Processes and Food, Beverages & Tobacco sectors have all comparable low levels of waste heat potential and also od diversity of waste heat streams (low temperature ones), the only appreciable exception being the Chemical Processes sector with a set of waste heat streams on the category of high temperature.

2.7.3. Categorisation of Process Industry Sectors

By the observation of the relative water and energy consumption levels presented in the section above, it is possible to perform a categorisation of each one of the approached sectors according to the relative uses of water and energy resources. In Table 2-14, the association of each one of the considered final energy consumption parcels (final energy, electricity, natural gas and oil), waste heat potential and water consumption for the case of the European Union are presented, while in Table 2-15 it is performed the classification of each one of the approached sectors in relation to each parcel according to the categorisation established in Table 2-14. A comparative analysis of the approached based on the established classification is presented in Table 2-16, and in Table 2-17 it is performed a comparison based on the GHG emissions levels presented in Figure 2.16.

Table 2-14. Categorisation of several sectors of the process industry in the European Union

Category	Final Energy (TJ/ (year.enterprise) and GWh/ (year.enterprise))				Waste heat (TJ/ (year.enterprise))	Water (dam^3/ (year.enterprise))
		Electricity	Natural Gas	Oil		
Low	0 – 40	0 – 6	0 – 14	0 – 0.5	0 – 15	0 - 90
Medium	40 – 80	6 – 12	14 – 28	0.5 – 1	15 – 30	90 – 180
High	80 – 120	12 – 18	28 – 42	1 – 1.5	30 – 45	180 – 270

Table 2-15. Classification of several sectors of the process industry in the European Union

Sectors		Final Energy				Waste heat	Water
			Electricity	Natural Gas	Oil		
Metal	Iron & Steel	Medium	Medium	Medium	Low	High	High
	Non-ferrous metals	High	High	High	High	Medium	
Non-metallic minerals	Cement & Lime	Low	Low	Low	Low	Low	
	Ceramic						
	Glass						
Paper & pulp		Medium	Low	Low	Medium	Low	Low
Textile		Low	Low	Low	Low		Low
Chemical Processes		Medium	Low	High	High	Medium	Medium
Food, Beverage & Tobacco		Low	Low	Low	Low	Low	Low

Table 2-16. Comparative analysis of Water and Energy Consumption Levels

Sectors		Analysis
Metal	Iron & Steel	• The average final energy consumption level parcels are associated to an overall medium level and are consistent with the absolute levels presented in Figure A2, signifying that the implementation of energy efficiency improvement measures is recommended to be analysed; • There is a relative high level of waste heat potential, signifying that the abovementioned implementation may be strongly analysed in terms of waste heat recovery.
Metal	Non-ferrous metals	• The average final energy consumption level parcels are associated to an overall high level, which are not consistent with the absolute levels presented in Figure A2 (signifying that each unit of this sector has a great representativity within the overall sector), signifying that the implementation of energy efficiency improvement measures is highly recommended to be analysed; • There is a relative medium level of waste heat potential, signifying that waste heat recovery may be a suitable a solution for the above-mentioned requirement.
Metal		• The relative high level of water consumption (which is consistent with the absolute values presented in Figure A2) signifies the adequacy of water recirculation studies and implementations, which may for instance be proceeded with heat-driven wastewater treatment (in the case of wastewater treatment requirements); • The sector has an overall medium necessity for water and energy efficiency improvement and high level of waste resources to be used for the purpose.
Non-metallic minerals	Cement & Lime Ceramic Glass	• The average final energy consumption level parcels are associated to an overall low level and are not consistent with the absolute levels presented in Figure A2 (signifying that each unit of this sector is not representative within the overall sector), signifying that the implementation of energy efficiency improvement measures is loosely recommended to be analysed; • There is a relative low level of waste heat potential; • The sector has an overall low necessity for energy efficiency improvement and low level of waste resources to be used for the purpose.
Paper & pulp		• The average final energy consumption level parcels are associated to an overall high level (which are consistent with the absolute levels presented in Figure A2) signifying that the implementation of energy efficiency improvement measures is loosely recommended to be analysed; • There is a relative low level of waste heat potential, signifying that waste heat recovery may only partially be a suitable option to be considered for energy efficiency improvement; • The relative low level of water consumption (which is consistent with the absolute values presented in Figure A2) signifies that water efficiency improvement is loosely recommended to be analysed; • The sector has an overall low necessity for water and energy efficiency improvement and low level of waste resources to be used for the purpose.
Textile		• The average final energy consumption level parcels are associated to an overall high level (which are consistent with the absolute levels presented in Figure A2) signifying that the implementation of energy efficiency improvement measures is loosely recommended to be analysed; • The relative low level of water consumption (which is consistent with the absolute values presented in Figure A2) signifies that water efficiency improvement is loosely recommended to be analysed; • The sector has an overall relatively low necessity for water and energy efficiency improvement.
Chemical Processes		• The average final energy consumption level parcels are associated to an overall medium level, with natural gas and oil consumption presenting more verifiable levels (which are partially consistent with the absolute levels presented in Figure A2), signifying that the implementation of energy efficiency improvement measures is recommended to be analysed; • There is a relative medium level of waste heat potential, signifying that the abovementioned implementation may be analysed in terms of waste heat recovery; • The relative medium level of water consumption (which is not consistent with the absolute values presented in Figure A2, potentially signifying that the units of the sectors present different levels of water use) signifies the adequacy of water recirculation studies and implementations, which may for instance be proceeded with heat-driven

	wastewater treatment (in the case of wastewater treatment requirements); • The sector has an overall medium necessity for water and energy efficiency improvement and medium level of waste resources to be used for the purpose.
Food, Beverage & Tobacco	• The average final energy consumption level parcels are associated to an overall high level (which are consistent with the absolute levels presented in Figure A2, signifying that each unit of this sector is not representative within the overall sector) signifying that the implementation of energy efficiency improvement measures is loosely recommended to be analysed; • There is a relative low level of waste heat potential, signifying that waste heat recovery may only partially be a suitable option to be considered for energy efficiency improvement; • The relative low level of water consumption (which is consistent with the absolute values presented in Figure A2) signifies that water efficiency improvement is loosely recommended to be analysed; • The sector has an overall relatively low necessity for water and energy efficiency improvement and low level of waste resources to be used for the purpose.

Table 2-17. Comparative analysis of GHG Emissions Levels

Sectors		Analysis
Metal	**Iron & Steel**	• The rate of decarbonisation has been average compared to other sectors in the time span of 1990 – 2020; • By the reference year of 2020, it presents a relatively higher level of $CO_{2,eq}$ emissions in relation to the other analysed sectors; • Such average rate and current relatively high $CO_{2,eq}$ emissions justify the exploitation of decarbonisation-related improvement measures.
	Non-ferrous metals	
Non-metallic minerals	**Cement & Lime**	• The rate of decarbonisation has been average compared to other sectors in the time span of 1990 – 2020, being higher than the one from the Iron & Steel; • By the reference year of 2020, it presents the higher level of $CO_{2,eq}$ emissions in relation to the other analysed sectors; • Such average rate and current relatively high $CO_{2,eq}$ emissions potentially justify the exploitation of decarbonisation-related improvement measures.
	Ceramic	
	Glass	
Paper & pulp		• The rate of decarbonisation has been slow compared to other sectors in the time span of 1990 – 2020; • By the reference year of 2020, it presents the lower level of $CO_{2,eq}$ emissions in relation to the other analysed sectors; • Such slow rate of decarbonisation (allied to the relatively high average energy consumption levels identified in Table 2-17) still justify the exploitation of decarbonisation measures.
Textile		
Chemical Processes		• The rate of decarbonisation has been fast compared to other sectors in the time span of 1990 – 2020, signifying that implemented decarbonisation measures have been effective; • By the reference year of 2020, it presents a relatively high level of $CO_{2,eq}$ emissions in relation to the other analysed sectors; • Such current relatively high $CO_{2,eq}$ emissions justify the continuation of the exploitation of decarbonisation-related improvement measures.
Food, Beverage & Tobacco		• The rate of decarbonisation has been slow compared to other sectors in the time span of 1990 – 2020; • By the reference year of 2020, it presents a relatively low level of $CO_{2,eq}$ emissions in relation to the other analysed sectors, although higher than Paper & pulp; • Such slow rate of decarbonisation still justify the exploitation of decarbonisation measures, so to secure the maintenance of relatively low GHG emission levels.

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3. Computational Tool and Methodology

In this chapter, the development details and inherent capacities of the two most relevant assets introduced in this work, the concept of Water and Energy Integration Systems (WEIS) and the ThermWatt computational tool, are described. The methodology framework is firstly described, being performed the relation between the aforementioned two assets. Such is followed by the extensive description of the methodology inherent to the WEIS, being performed a comparison of this methodology with existing ones used in the context of process integration research for water and energy use improvement. The ThermWatt tool (which subsists on a set of simulation and optimisation models) is extensively described, with each one of the process industry equipment-level models included in the tool being characterized in terms of physical phenomena modelling. These models are submitted to a validation procedure performed through the comparison of simulation results with gathered real data, which is furtherly presented.

A set of scientific publications by the authors extensively detail the development aspects associated to the computational models of specific components [367–369].

3.1. Methodology Framework

The methodology adopted in this work shall be set for the definition and further use of the general innovative concept of Water and Energy Integration Systems (WEIS). These may be defined as complex installations to be installed in end-use sector facilities set to perform the maximum use of the recirculation of energy (mainly waste heat) and water streams for the purpose of causing an overall eco-efficiency promotion, encompassing the conjoined benefits of energy savings, water savings and solid and gas contaminant reduction and overall economic benefits. These systems are based on the installation of a set of technologies that may be used in the context of the exploitation of the interdependencies of energy and water resources [33], such as the ones extensively approached in chapter 2.

The analysis of the implementation of these types of systems may be performed in a virtual basis through the use of computational models, which in this work is handled through the development and use of the ThermWatt computational tool. The computational models developed using the capacities of this tool allow the analysis of a plant from a departing point (in which significantly high energy use, water use and pollutant emissions are verified and none or few improvement measures are implemented) to an end point (corresponding to the reduced use of resources and emissions).

The aim of the use of ThermWatt in the context of this work is the virtual implementation of WEIS in industrial case-studies. For such implementation, the first step is the development and use of simulation models (system-level models which encompass several interconnected component-level models corresponding to the industrial processes and improvement technologies), which is performed using the object-oriented modelling language Modelica, namely the open-source environment OpenModelica. The simulation tool allows in this sense the assembling of a WEIS flowsheet. Several scenarios may be created based not only on several different points of stream recirculation but also on the installation of several analogous technologies. Such takes part of the overall scenario analysis procedure, which allows to select the most favourable scenarios for each targeted case-study. For the further analysis procedures, only one of these scenarios will be selected for each case-study. The overall performance of the simulations is set to allow the assembling of WEIS superstructures adapted to the case-studies by the establishment of the several different scenarios and to obtain primary improvement results.

The obtained results are nonetheless still associated to an uncertainty regarding its consideration of being the optimal scenarios (in which the eco-efficiency of the plant is the highest possible within the implementation of the conceptualized WEIS). As such, an optimisation procedure is undertaken, subsisting on the development of an optimisation model which serve as counterparts to the previously developed simulation models. According to the specific modelling requirements, these models are developed using two different languages: the Python language for steady-state perspective ones (namely the ones using the linear, non-linear, mixed-integer linear, mixed-integer non-linear and multi-objective programming methodologies) and Modelica for transient-based ones (namely through the use of the OpenModelica *optimization* solver for the development of a model applying the dynamic programming methodology). In the case of the models developed in the Python language, the respective optimisation results are set to be integrated in the counterpart Modelica simulation models using the OpenModelica Python API [370]. In the case of the latter models, such direct integration is not directly possible, due to inexistence of a proper API that connects the Modelica models developed to be used with the *optimization* solver and the counterpart simulation models (developed with the DASSL solver). The running of these models allows for the achievement of optimised results for the WEIS considering the aim of maximum eco-efficiency promotion (which in practice is set to be formulated as the minimization of the summation of all annualized costs parcels). These ultimate WEIS scenarios have significantly reduced water use, energy use and pollutant emission in comparison to the baseline scenario.

Taking into account a potentially still existing uncertainty of the final results (which in this case is accounted by the non-consideration of determinate aspects which have been considered to be subjective in the formulation of the mathematical models), a set of key performance indicators (such as the ones exploited in section 2.6) are set to be calculated. In a post-processing view, these are set to ultimately evaluate the economic and environmental impact mitigation performance of the conceptualized installation.

In Figure 3.1, the general methodology inherent to this work is schematically presented.

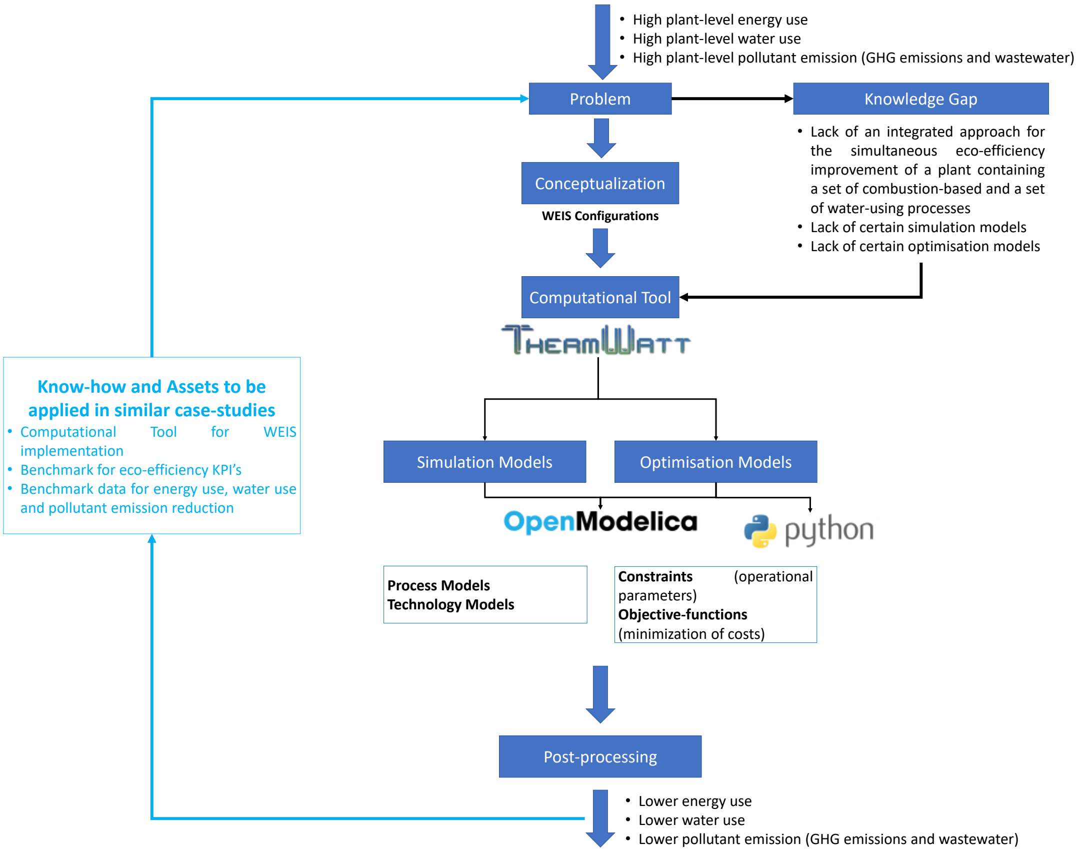


Figure 3.1. Schematic of the methodology encompassing both the ThermWatt tool and the WEIS concept

3.1.1. Application of the Water and Energy Integration Systems (WEIS) Concept

The presented modelling framework is set for the virtual implementation of WEIS configurations in existing industrial sites. Each one of the developed models is purposed to include a part of the existing industrial processes of the plant (namely combustion-based processes and water-using processes) and a set of unit operations that are part of a project for the improvement of resources in a plant (the technologies or units to be implemented). In Table 3-1, it is presented a general setup of the simulation and optimisation models to be considered for the virtual implementation of WEIS.

Table 3-1. General setup of simulation and optimisation models for WEIS

Model Aspect	Specifications
Component-level simulation models and inherent phenomena	• Combustion-based process models (Mass and enthalpy balances); • Water-using process models (Mass and enthalpy balances); • Improvement technologies: ○ Heat recovery including thermal energy storage (Mass balances, enthalpy balances, heat transfer and reaction); ○ Heat-driven wastewater treatment (Mass balances, enthalpy balances and heat transfer);

	○ WWtE units including TWS (Mass balances, enthalpy balances, heat transfer and reaction).
Optimisation models inequality constraints	For Water system-side: • Maximum contaminant concentration (inlet and outlet of WP's and WWT units); • Maximum water flow rate (inlet of WP's). For Thermal process system-side: • Maximum inlet combustion air temperature; • Minimum condensation temperature of exhaust gases; • Maximum flow rate of recirculated waste heat stream (in the case of hot air streams which a part of the total flow rate must be recirculated for space heating).
Optimisation models equality constraints	• Mass balance equations; • Enthalpy balance equations; • Heat transfer equations.
Optimisation models objective functions	Minimization of total costs including: • CAPEX (which shall be annualized); • OPEX (additional costs for maintenance and utilities); • Water costs; • Energy costs; • Emissions costs.

3.1.2. Comparison to the Combined Water and Energy Integration (CWEI) and Total Site Integration (TSI) Methodologies

Attending that the WEIS concept attempts for a plant-wide process integration including in the limit all the processes of the same categories, its inherent methodology may be compared to other PI methodologies which aim for the consideration of a high number of processes. These are mainly the Combined Water and Energy Integration (CWEI) and Total Site Heat Integration (TSI). In Table 3-2, it is performed a comparison of these methodologies.

Table 3-2. Comparison of Process Integration Methodologies (CWEI, TSI and WEIS)

Existing Methodologies	Water and Energy Integration Systems (WEIS) Methodology
Combined Water and Energy Integration (CWEI) • The object of study is a water network constituted by a set of water-using processes and wastewater treatment units; • It is based on the application of steady-state based optimisation methodologies for the assessment of the most favourable levels of water stream recirculation in several points of the water network; • Being based on the use of a resource as both an additional water and heat source, it only considers water streams for recirculation. **Total Site Integration (TSI)** • The object of study is a set of energy-using	• The object of study is a set of water-using and combustion-based thermal processes within a plant; • It is based on the assessment of all potential recirculation points of discharge water and heat streams; ○ Heat streams may be recirculated to all thermal processes (independently from the process of origin), thermodynamic cycles to be installed, the heaters of the water system and the heat-driven wastewater treatment units; ○ Discharge water streams (with variable concentration of contaminants, according to the

processes connected by a common utility system; • It is based on the analysis of heat recovery between several processes through consumption and generation of utilities, in each the heating and cooling needs of each process are identified for the purpose of utility targeting; • The supply of utilities with the aim to improve energy use may be performed through several measures (utility replacement, recirculated heat streams and renewable energy resources); • For variable energy demand and supplies, it may involve the use of thermal energy storage units; • It is itself an extension of the simpler heat integration methodologies (such as pinch analysis).	point of origin) may be recirculated from one unit operation of one water-using line to the inlet of the others within the same line and to the inlet of all the processes within the other water-using lines. • The practical method is based on the valorisation of output streams, rather than on the rationalization of input streams; • In terms of technological integration, it overall encompasses the same technologies as CWEI and TSI and in addition wastewater-to-energy units.

As may be evidenced by the analysis presented in Table 3-2, the innovative methodology inherent to WEIS implementation may be considered a simultaneous expansion and combination of the CWEI and TSHI methodologies in conceptual terms. For instance, it overall considers categories of processes that are not considered in CWEI (it only considers water-using processes and associated consumption of material and energy-related utilities) and TSI (its scope is summed up to energy-using processes and related utility system).

The CWEI is essentially encompassed within the general concept of WEIS, and as such the improvement potential of water networks is the same for CWEI and the WEIS. While the TSI does not only consider energy efficiency improvement based on energy recovery methods but also on the adaptation/ substitution of energy inputs, the general concept of WEIS considers system-level improvements only through discharge stream recirculation (which would otherwise be classified as several types of wastes). Nonetheless, the WEIS concept does not completely disregard the consideration of other energy inputs (such as renewable resources and alternative hot and cold utilities), it only focuses on waste stream valorisation. Such conceptual option is set to maximize solely the valorisation of otherwise waste streams generated in a plant (so to minimize energy inputs only through the maximization of the recirculation of to-be-valorised streams).

3.1.3. Conceptualization of Water and Energy Integration Systems (WEIS)

In general, the conceptualization of Water and Energy Integration Systems (WEIS) passes by the simultaneous application of the principles of water recirculation and heat recovery [6–8]. In this prospect, two different configurations have been primarily conceptualized:

- **Configuration 1**: Standard Configuration (encompassing combustion-based process in continuous operation only and a general steady-state perspective);
- **Configuration 2**: Dynamic Configuration (encompassing combustion-based process in continuous and batch operation, the implementation of thermal energy storage units a general transient-state perspective).

The conceptualization of a WEIS may be overall characterized by the following sequence of steps:

- The use the waste heat potential from a discharge stream from a combustion-based process for the purpose of the reduction of fuel consumption in a set of combustion-based processes [369];
- The use the waste heat potential from a discharge stream from a combustion-based process for the purpose of the electricity generation through the installation of thermodynamic cycles [369];
- The recirculation of a set of water streams to produce savings in freshwater consumption [347];
- The recirculation of a set of water streams in the context of the use of its waste heat potential to produce savings in the hot utilities used in specific points of a water system (heaters) [6];
- The recirculation of a set of water streams produce savings in the cold utilities used in specific points of a water system (coolers) [6];
- The use the waste heat potential from a discharge stream from a combustion-based process to set the operation of a water treatment and recirculation system (in the case of heat-driven water treatment [11]);
- The use of the discharge water streams and discharge sludge streams from a wastewater treatment unit for the production of additional fuels in wastewater-to-energy units [85].

The general description points associated to all superstructures may be extensively defined as follows:

- The WEIS encompasses M combustion-based processes and N water-using processes;
- Each combustion-based process encompasses the feeding of a fuel stream (primary energy source) and combustion air stream;
- Each combustion-based process encompasses a set of waste heat streams, which jointly constitute a potentially recirculated heat stream (to the same process or other processes);
- The set of all combustion-based processes and its inlet and outlet streams constitutes the designated thermal process system;
- The set of a combustion-based process and recirculated heat streams that are transported from the outlet to the inlet of processes constitute a thermal process sub-system;
- In the context of the superstructures furtherly represented, the recirculated heat stream directed to a combustion-based process's inlet may (direct heat recovery) or may not (indirect heat recovery) be mixed with the inlet ambient air stream (it depends whether the recirculated heat stream is air or an exhaust gas, as commonly verified and implemented);
- The recirculated heat stream at the outlet of a combustion-based process may be recirculated to the same combustion-based process or the other M – 1 combustion-based processes;

- In Configuration 2, another recirculated heat stream is transported to an energy storage system (TES) to heat up a heat sink stream, which is then split to be fed to each combustion-based processes;
- For each water-using process is installed a WWT unit for the treatment of the wastewater stream at the outlet of the water-using process, in addition to a heater and a cooler;
- The set of all water-using processes, WWT units, heater, cooler and inlet, outlet and recirculated streams constitutes the water system;
- The set of a water-using process, associated WWT unit, heater, cooler and respective inlet, outlet and recirculated streams (which do not recirculate to other N – 1 water-using processes) constitute a water sub-system;
- Each water sub-system is fed by a freshwater stream and a discharged water stream results as an outlet stream;
- At the outlet of the water-using process, WWT unit, heater and cooler results several recirculated streams (recycled, reused and by-passed):
    - From the water-using process to the WWT unit inlet, heater inlet, cooler inlet, the WS outlet, other N – 1 heaters and other N – 1 coolers;
    - From the WWT unit to WP inlet, heater inlet, cooler inlet, the WS outlet, other N – 1 heaters and other N – 1 coolers;
    - From the heater to WP inlet, WWT unit inlet and WS outlet;
    - From the cooler to WP inlet, WWT unit inlet and WS outlet;
    - For each WWT unit, a sludge stream is generated and then directed to the inlet of a wastewater-to-energy module (mixed with the discharged water stream);
    - The generated energy (in the form of fuel) in the wastewater-to-energy is directed to the inlet of each combustion-based process sub-system and a combustion chamber which is (by hypothesis) installed within the thermodynamic cycle;
    - In the context of the configuration furtherly represented, the additional fuel stream may be (directly) mixed with the primary fuel stream or be (indirectly) transported to each combustion chamber.
- In addition to the recirculation within the thermal process system, the recirculated heat may be directed to the water system (the stream is divided for each water sub-system, and in its turn for each heater and WWT unit), a thermodynamic cycle (for the production of additional electric energy) and the WtE unit (according to the specific energy input in this process);
    - The generated electricity is directed to each WWT unit and the WtE unit.

The configurations for a thermal process system (Configuration 1 not including and Configuration 2 including a thermal energy storage unit) and a water system are presented in Figures 3.2 – 3.3 (in the form of abridged concepts) respectively and Figures 3.4 – 3.6 (the actual general superstructures corresponding to each configuration) respectively. Two different configurations (1 and 2) defining WEIS are presented in Figure 3.7 and 3.8. The nomenclature to identify each stream in the aforementioned figures is described in Table 3-3.

Table 3-3. Elaborated notation in respect to the streams encompassed in Water and Energy Integration Systems (WEIS)

Abb.	Description	Abb.	Description
Ai	Ambient air stream at the inlet of combustion-based process sub-system i	rTWoi,j	Recirculated treated water stream from wastewater treatment unit I to water sub-system j
Aei	Additional energy source generated from waste-to-energy unit i	rTWoi,j,c	Recirculated treated water stream from wastewater treatment unit I to cooler j
ATPEi	Additional energy allocated to combustion-based combustion-based process i	rTWoi,j,h	Recirculated treated water stream from wastewater treatment unit I to heater j
ATC	Additional energy allocated to thermodynamic cycle system	rWWci	Recirculated wastewater stream from water-using process to cooler i
bFWfi	Freshwater stream allocated from the water sub-system inlet to the outlet of the same sub-system i	rWWhi	Recirculated wastewater stream from water-using process to heater i
bFWTi	Freshwater stream allocated from the water sub-system inlet to the inlet of the wastewater treatment unit i	rWWoi,j	Recirculated wastewater stream from water-using process I to water sub-system j
bWWfi	Wastewater stream allocated from water-using process to the outlet of water sub-system i	rWWoi,j,c	Recirculated wastewater stream from water-using process I to water cooler j
Ci	Inlet contaminant in water-using process i	rWWoi,j,h	Recirculated wastewater stream from water-using process I to water heater j
CAi	Combustion air at the inlet of combustion-based process i	RHi	Recirculated heat source stream from combustion-based process i
CCi	Combustion chamber from combustion-based process i	RHi,j	Recirculated heat source stream from combustion-based process i to combustion-based j
CTC	Combustion chamber from thermodynamic cycle	RHE	Recirculated heat source stream to thermodynamic cycle
CUi	Cold utility allocated to cooler i	RHHi	Recirculated heat source stream to heater i
DS	Discharge stream from water system	RHTES	Recirculated heat source stream from combustion-based process sub-system to the thermal energy storage unit
DWi	Discharged water stream from water sub-system i	RHTPi	Recirculated heat source stream from thermal energy storage unit to combustion-based process i
E	Electric energy generated in the thermodynamic cycle	RHTPWS	Recirculated heat source stream from thermal energy storage unit to combustion-based process system, water system and thermodynamic cycle
FW	Freshwater stream at the inlet of the whole water system	RHWtE	Recirculated heat to the wastewater-to-energy unit
FWi	Freshwater stream at the inlet of the water sub-system i	RHWS	Recirculated heat source stream to water system
HUWCi	Water stream at the outlet of cooler i	RHWSi	Recirculated heat source stream from combustion-based process i to water system (and thermodynamic cycle)
HUWHi	Water stream at the outlet of heater i	RHWWTi	Recirculated heat source stream to wastewater treatment unit i
HSTES	Heat sink stream to thermal energy storage unit	sFWi	Separated freshwater stream at the inlet of water sub-system i
HSTESTP	Heat sink stream at the outlet of the thermal energy storage unit	sTWi	Separated treated water stream at the outlet of water sub-system i
HSTESTPi	Heat sink stream from the thermal energy storage unit to combustion-based process i	sWWi	Separated wastewater stream at the outlet of water-using process i

Table 3-3. Elaborated notation in respect to the streams encompassed in Water and Energy Integration Systems (WEIS) (Cont.)

Abb.	Description	Abb.	Description
HUi	Hot utility allocated to heater i	Si	Sludge stream at the outlet of wastewater treatment unit i
PE	Fuel stream at the inlet of the combustion-based process system	TES	Thermal Energy Storage unit
PEi	Fuel stream at the inlet of combustion-based process sub-system i	TPi	Combustion-based process i
rFWci	Freshwater stream allocated from the water sub-system inlet to cooler i	TC	Thermodynamic cycle
rFWhi	Freshwater stream allocated from the water sub-system inlet to heater i	uWi	Feed water stream at the inlet of water-using process i
rhuWcfi	Recirculated wastewater stream from cooler to the outlet of water sub-system i	uWWi	Feed wastewater stream at the inlet of wastewater treatment unit i
rhuWhfi	Recirculated wastewater stream from heater to the outlet of water sub-system i	uWci	Feed wastewater stream at the inlet of cooler i
rhuWcPi	Recirculated wastewater stream from cooler to the inlet of water sub-system i	uWhi	Feed wastewater stream at the inlet of heater i
rhuWhPi	Recirculated wastewater stream from heater to the inlet of water sub-system i	uWphi	Feed wastewater stream at the inlet of water pre-heater i
rhuWcTi	Recirculated wastewater stream from cooler to the inlet of wastewater treatment unit i	WAE	Stream at the inlet of the wastewater-to-energy unit
rhuWhTi	Recirculated wastewater stream from heater to the inlet of wastewater treatment unit i	WH	Waste heat stream from overall system
rTWi	Recirculated treated water stream from wastewater treatment unit to the inlet of water sub-system i	WHE	Waste heat stream from thermodynamic cycle
rTWci	Recirculated treated water stream from wastewater treatment unit to cooler i	WHHi	Waste heat stream from heater i
rTWhi	Recirculated treated water stream from wastewater treatment unit to the heater i	WHTES	Waste heat stream at the outlet of the thermal energy storage unit
Elec	Net generated electricity	WHWtE	Waste heat stream from wastewater-to-energy unit
ElecWWTi	Electricity directed to wastewater treatment unit i	WHWWTi	Waste heat stream from wastewater treatment unit i
ElecWtE	Electricity directed to the wastewater-to-energy unit	WtE	Wastewater-to-energy unit
S	Sludge stream at the outlet of water system	WWTi	Wastewater treatment unit i

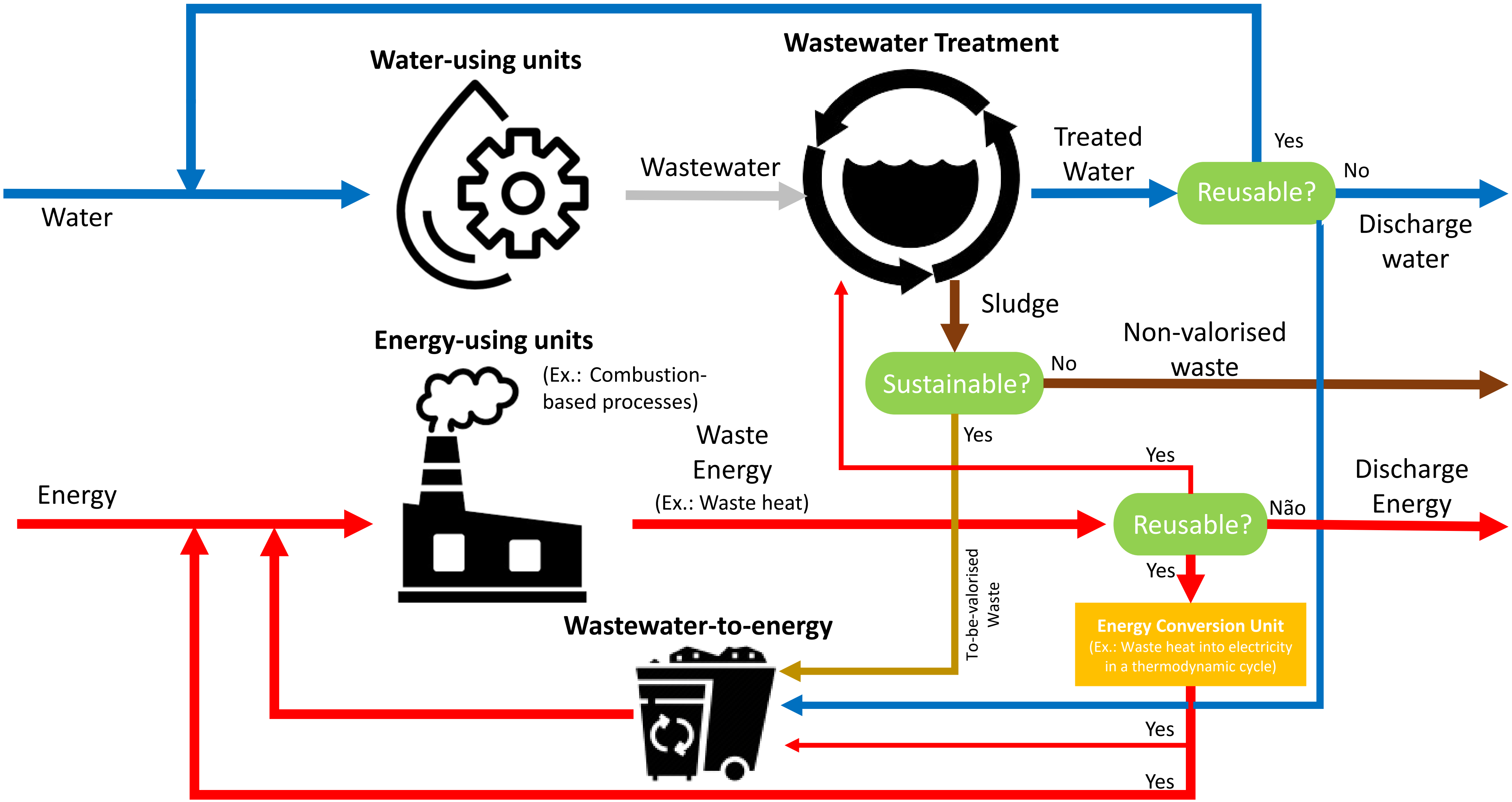


Figure 3.2. Abridged concept for WEIS Configuration 1 (Standard)

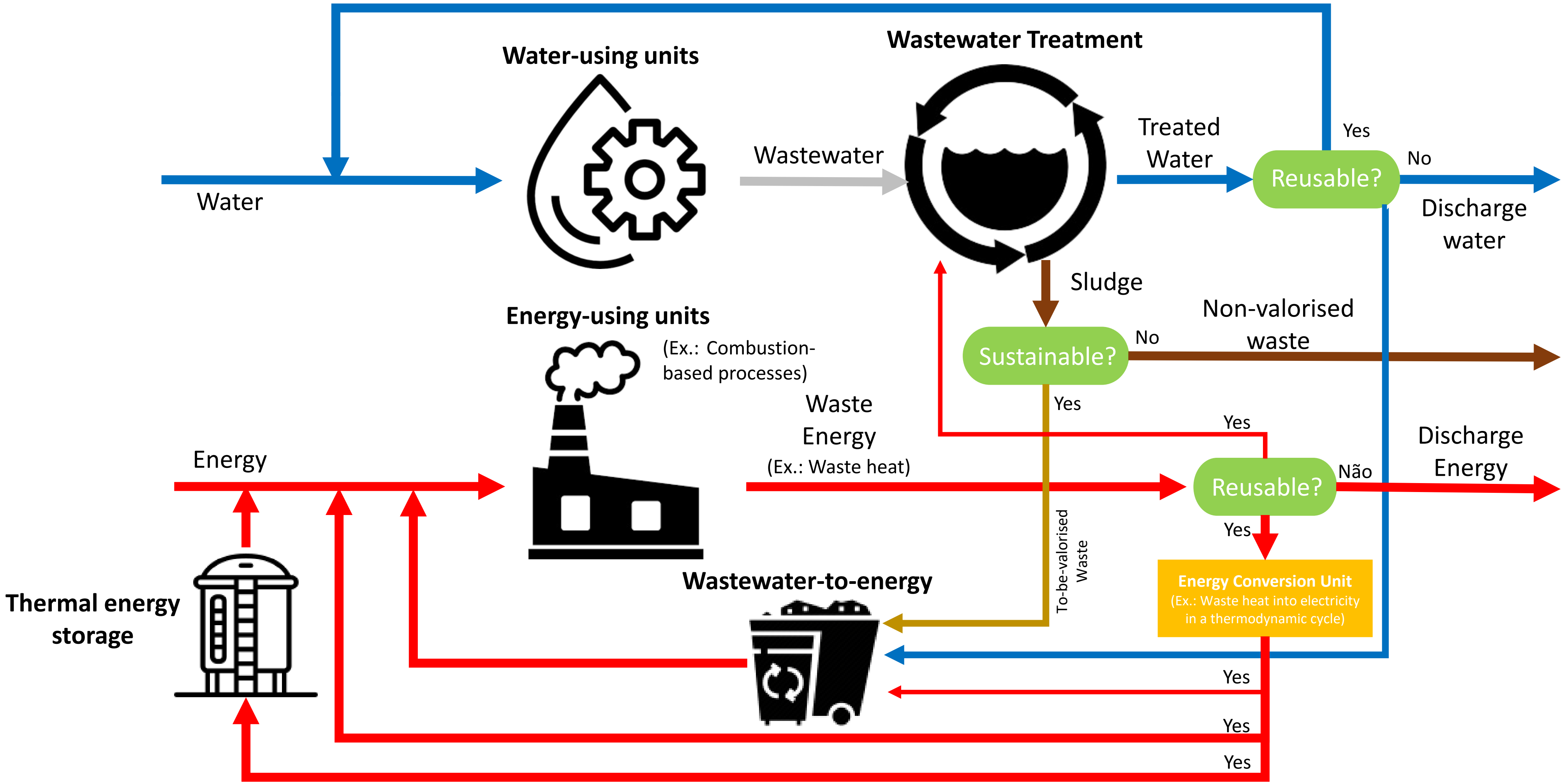


Figure 3.3. Abridged concept for WEIS Configuration 2 (Dynamic)

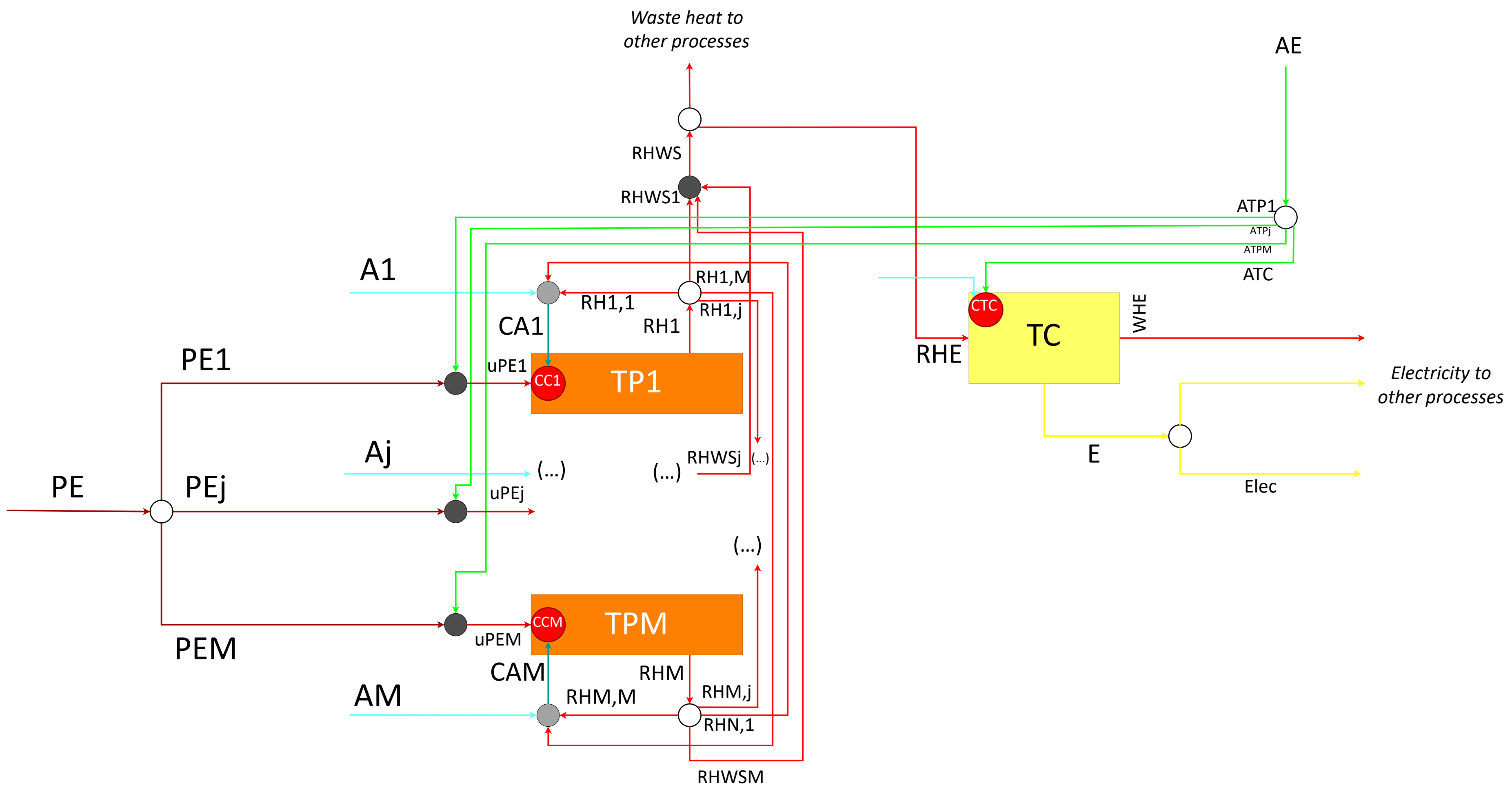


Figure 3.4. Generalized superstructure for a Thermal Process System (Standard), in which black-filled circles (●) represent stream mixing, grey-filled circles (◎) represent ambiguous stream mixing (in this case, these are used to represent that the recirculated heat stream may be recirculated either as pre-heated air to be mixed with ambient air or to an air preheater (exiting as a waste heat stream)) unfilled circles (○) represent stream splitting

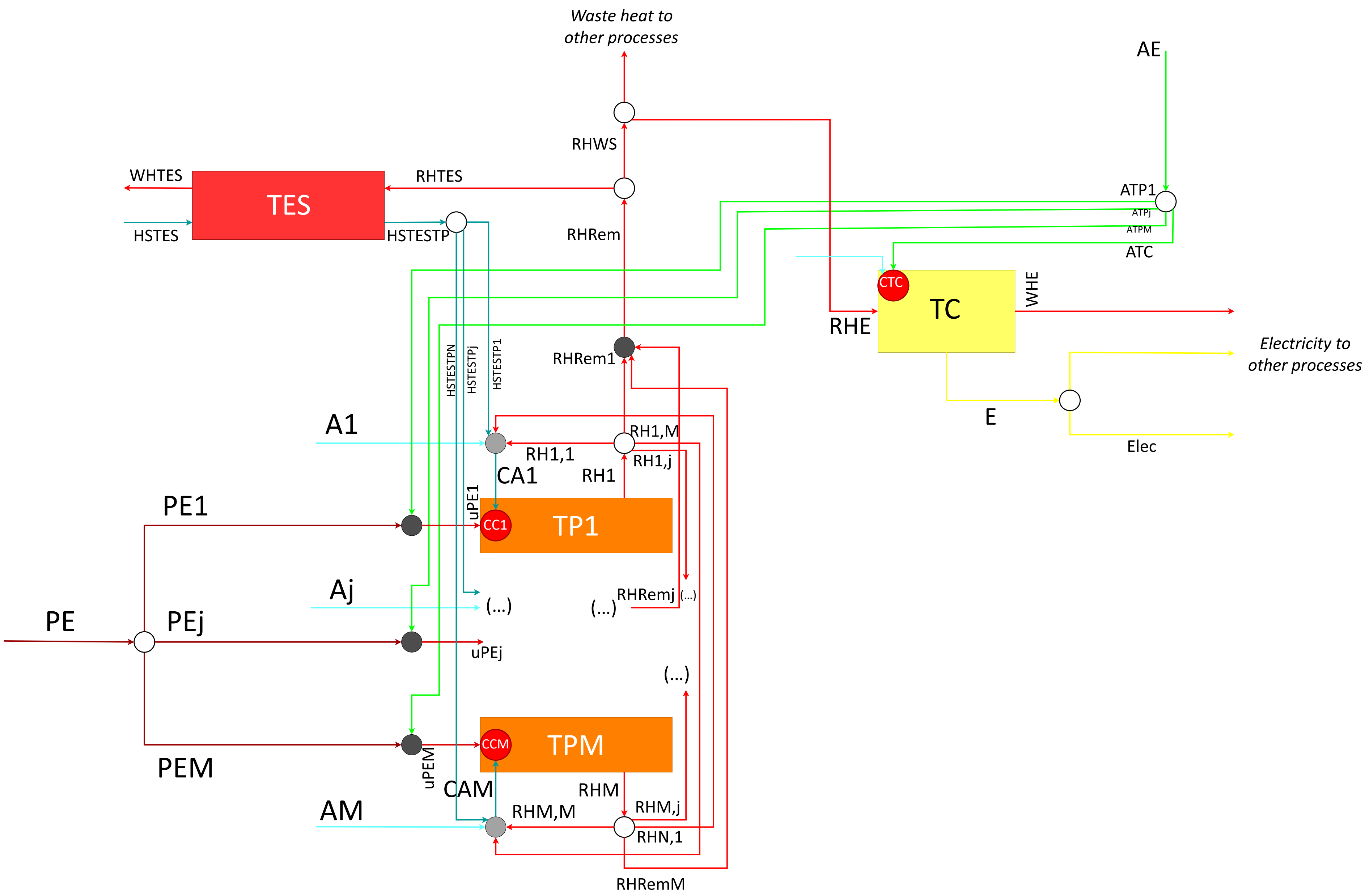


Figure 3.5. Generalized superstructure for a Thermal Process System (including a Thermal Energy Storage unit)

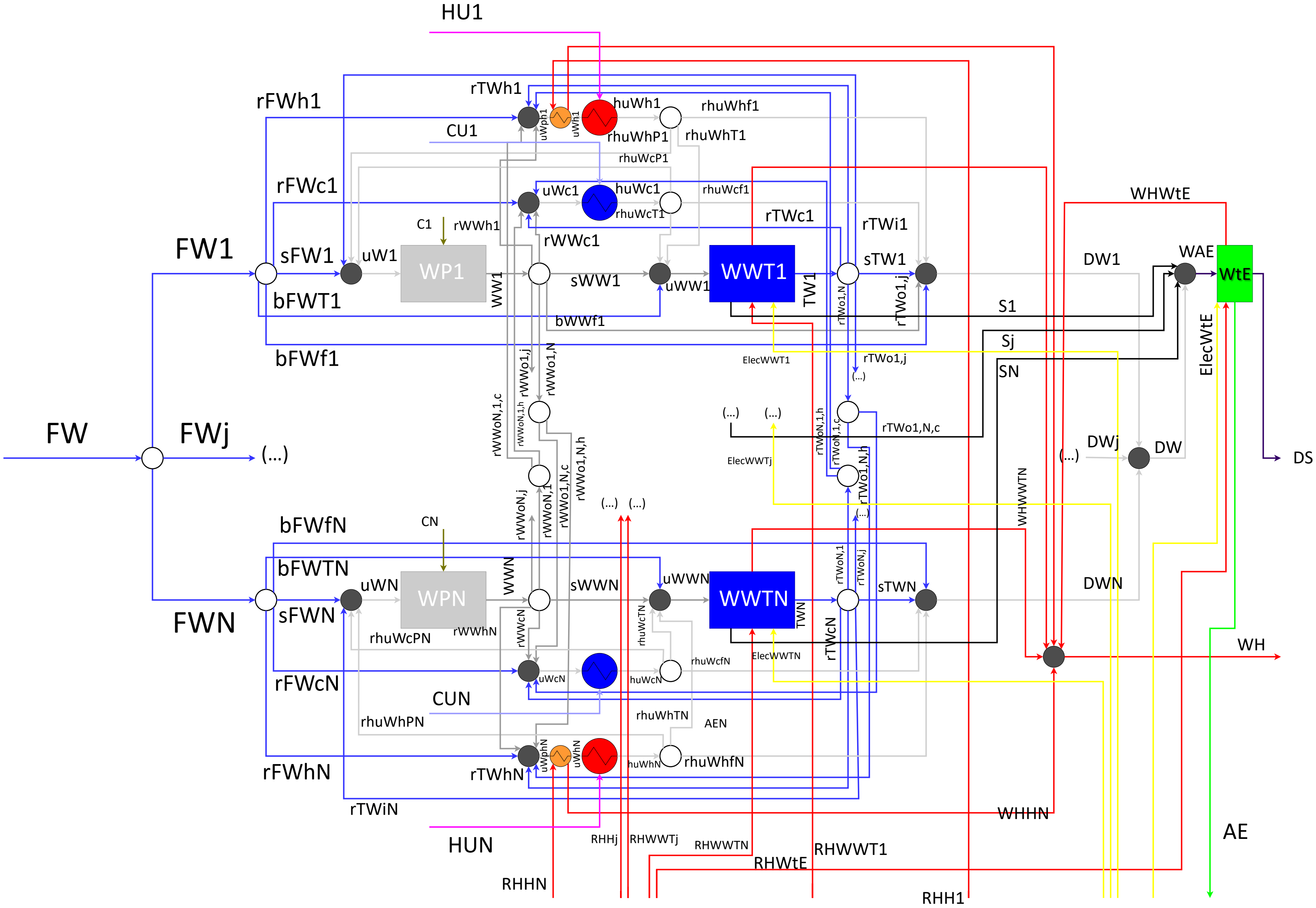


Figure 3.6. Generalized superstructure for a Water System

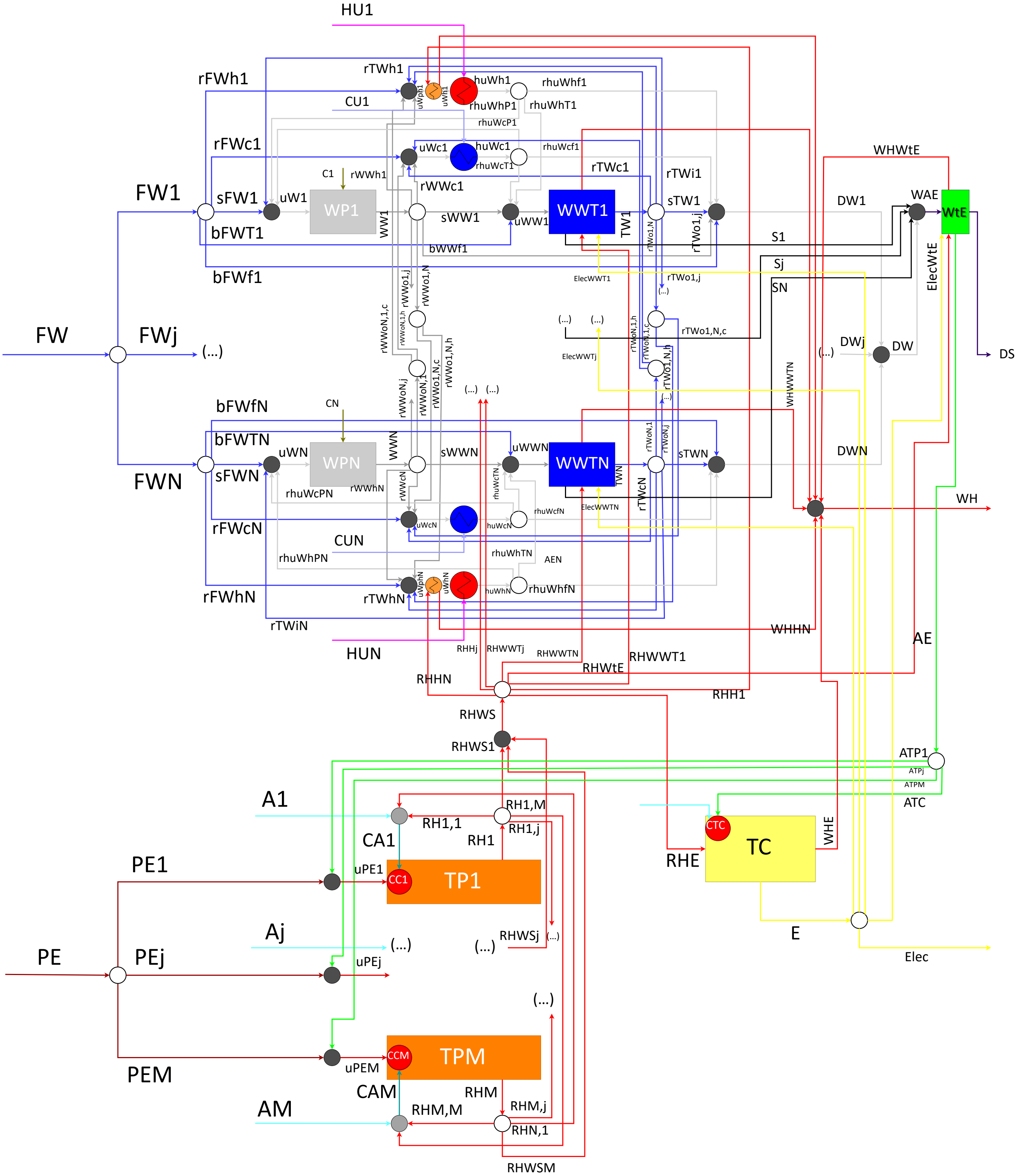


Figure 3.7. Generalized superstructure for WEIS Configuration 1 (Standard)

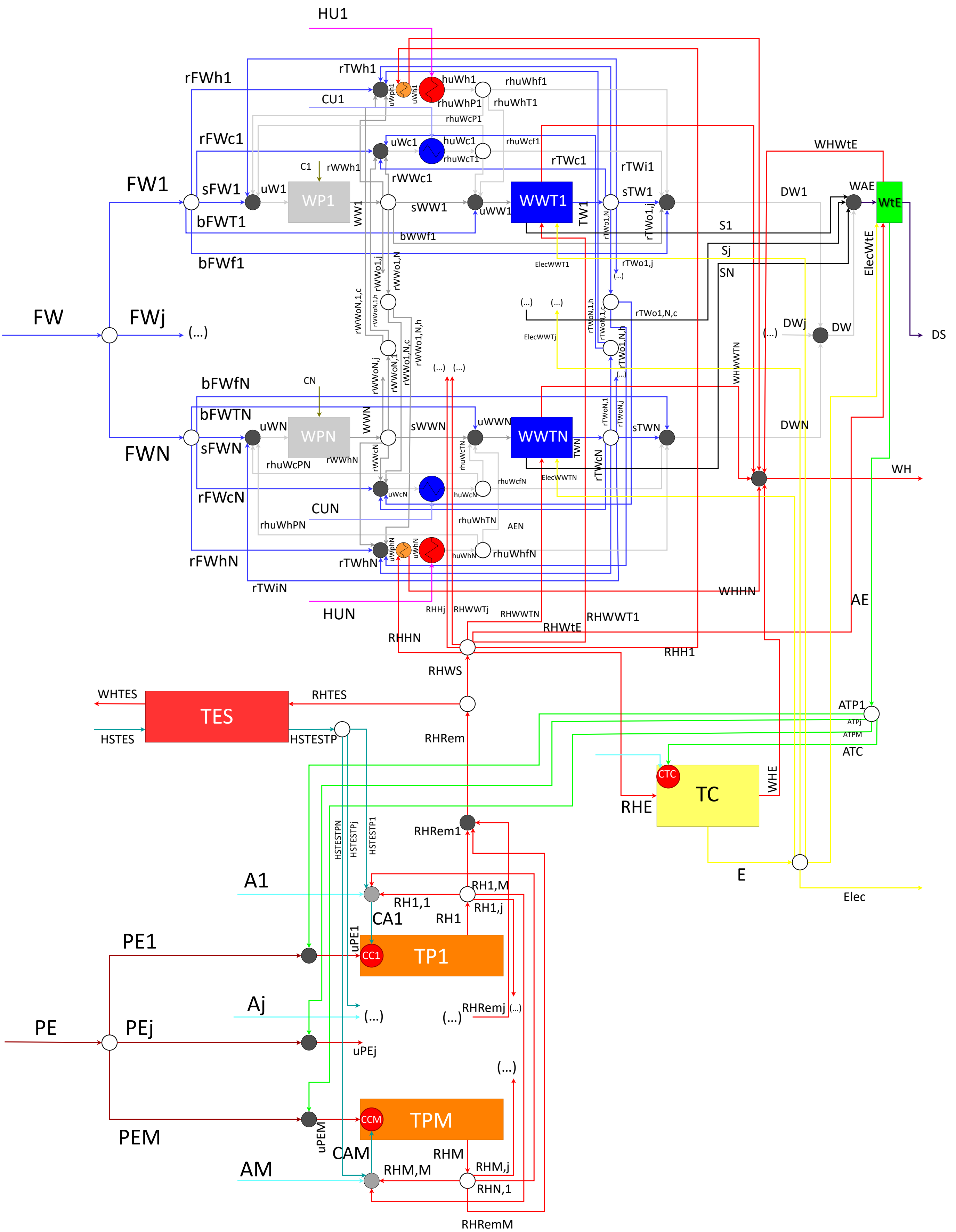


Figure 3.8. Generalized superstructure for WEIS Configuration 2 (Dynamic)

3.2. Conceptualization of Simulation Models

The simulation models on the scope of this work are constructed by gathering of a set of equations characterizing the physical phenomena occurring in each one of the considered unit operations. The occurring phenomena exploited on the scope of this work may be generally classified into thermal phenomena (relative to changes in temperature and specific enthalpy), hydraulic phenomena (relative to changes in pressure) and reaction phenomena (involving a chemical reaction). Furthermore, a set of equations must be set for the consideration of the phenomena of splitting and mixing of fluid streams. The most general categories of model development in this section are divided (by a reason of convenience) into:

- Modelling of Heat Recovery and Water Recirculation Phenomena (approaching the basic operation of heat recovery and water recirculation);
- Modelling of Heat Recovery Technologies (approaching the phenomena of heat transfer occurring in heat recovery devices);
- Modelling of Heat-Driven Wastewater Treatment Units (approaching the phenomena of heat transfer from a heat sour stream to a wastewater stream for the purpose of producing treated water);
- Modelling of Wastewater-to-energy Technologies (approaching the reaction phenomena which involves the conversion of discharge water and wastewater streams with suitable content into additional fuel).

3.2.1. Modelling of Heat Recovery and Water Recirculation Phenomena

The phenomena of heat recovery and water recirculation consist of the basic occurrence of stream recirculation, which is in practice performed to permit the decrease of the input of freshwater and/ or energy (fuels and hot/ cold utilities). Such phenomena subsist on the most general mass and enthalpy equations represented in Table 3-4.

Table 3-4. General mass and enthalpy balance for stream recirculation

Phenomenon		Equation	
Splitting	Mass balance	$\dot{M}_{in} = \sum_{i=1} \dot{M}_{out,i}$	(3.1)
	Enthalpy balance	$h_{in} = h_{out,i}$	(3.2)
Mixing	Mass balance	$\sum_{i=1} \dot{M}_{in,i} = \dot{M}_{out}$	(3.3)
	Enthalpy balance	$\sum_{i=1} \dot{M}_{in,i} \cdot h_{in,i} = \dot{M}_{out} \cdot h_{out}$	(3.4)

It is to note that the specific enthalpy (h) and the temperature (T) of a medium are variables that depend one from the other according to a relation that it is proper to each medium, as generally enunciated in Table 3-5.

Table 3-5. General relations between specific enthalpy, specific heat capacity and temperature variables

Category		Equation	
Specific Enthalpy – Temperature relation		$h = f(T)$	(3.5)
Specific heat capacity – Temperature relation	**Single phase**	$\frac{dh}{dT} = C_P$	(3.6)
	Phase change	$\frac{dh}{dT} = C_{P,app}$	(3.7)

The formulations performed in this work tendentially use the form of the respective equations that use specific enthalpy (h) rather than temperature (T), except on the case of heat transfer equations, by a reason of convenience. It is to note that a different generic designation is used for the specific heat capacity for single phase (C_P) and phase change ($C_{P,app}$). In this case, the first is used to designate a specific heat capacity variables which is associated to only slight variations with temperatures (which is the case for within a same physical phase) and the latter for specific heat capacity variables with high variations with temperature (as it is verified in phase change, in the limit taking the value of infinite due to the inexistence of the variation of temperature with specific heat capacity for certain media).

The splitting and mixing phenomena-related equations presented in Table 3-4 are set to be adapted for each the cases of heat recovery and water recirculation in particular.

i) Modelling of Heat Recovery and Combustion-based Thermal Processes

The principle of heat recovery may be explained by the reduction of fuel consumption considering the same supplied heat [371]. In its turn, the total supplied heat (q_{supply}) may be calculated considering the fuel's lower heating value (LHV), attending to equation (3.8), in which $\dot{M}_{Fuel_{Baseline}}$ is the fuel consumption of a combustion processes (or a set of combustion processes) for the baseline scenario. For the case in which more than one heat source exists to supply thermal energy to processes (in the case that a heat recovery system has been implemented), it is necessary to consider an additional heat parcel ($q_{additional}$), as described by equation (3.9). The additional heat ($q_{additional}$) depends on the combustion process that is being analysed, and as such may defined for different cases. The set of equations (3.8) and (3.9) were in this case enunciated adapting the equations proposed by Tangjitsitcharoen et al. [371] for waste heat recovery based on the implementation of high efficiency burners for a general case.

$$q_{supply} = \dot{M}_{Fuel_{Baseline}} \bullet LHV \tag{3.8}$$

$$q_{supply} = \dot{M}_{Fuel} \bullet LHV + q_{additional} \tag{3.9}$$

The $q_{additional}$ may be determined through the calculation of the enthalpy allocated from waste heat stream, whose mixing and recirculation phenomena is expressed by an adapted set of equations from Table 3-4. For direct stream recirculation (for instance, in the case that hot air is mixed with ambient air to form combustion air) this parcel may be determined by direct adaption of the mixing phenomena equations from Table 3-4. In the case such enthalpy allocation is performed indirectly (for instance, through heat transfer from exhaust gases to the inlet combustion air), the enunciation of this parcel is different. The definition of the $q_{additional}$ parcel according to these two cases is presented in Table 3-6.

Table 3-6. General mass and enthalpy balance for stream recirculation

Phenomenon	Equation	
Direct Allocation of Enthalpy	$q_{additional} = \dot{M}_{recirc.stream} \bullet (h_{recirc.stream} - h_{Baseline})$	(3.10)
Indirect Allocation of Enthalpy	$q_{additional} = eff_{HT} \bullet \dot{M}_{recirc.stream} \bullet (h_{recirc.stream,in} - h_{recirc.stream,out})$	(3.11)

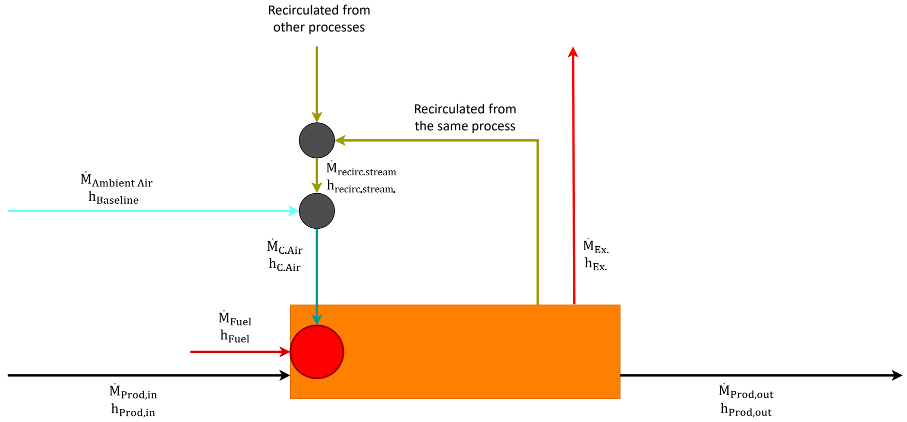
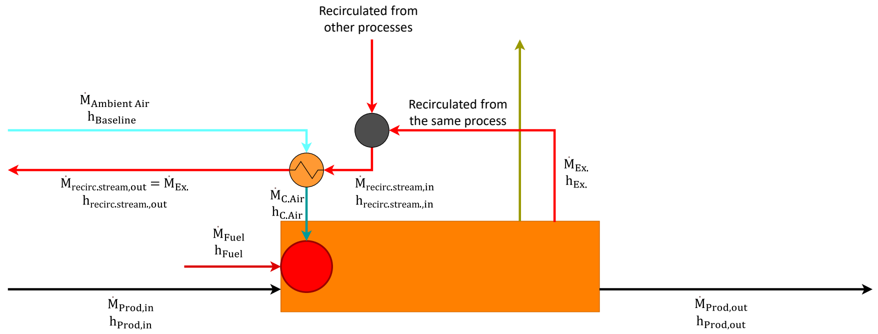
The heat recovery phenomenon occurs nearby the combustion-based processes. The mass and enthalpy balances within a process of this type is influenced by the different levels of fuel and combustion air input (input mass flow rate and temperature), being that the conditions of the outlet streams (namely, exhaust gases and produced material) vary with different sets of those conditions. The general mass and enthalpy equations for a combustion-based process are presented in Table 3-7.

Table 3-7. Mass and Enthalpy Balance equations for a Combustion-based Process

Zone	Equation		
Combustion Chamber	Mass Balance	$\dot{M}_{Fuel} + \dot{M}_{C.Air} = \dot{M}_{ExGas}$	(3.12)
	Enthalpy Balance	$\dot{M}_{Fuel} \bullet (h_{Fuel} + LHV) + \dot{M}_{Air} \bullet h_{Air} = q_{reac.}$	(3.13)
Heating Zone (Serving for the achievement of the purpose of the installation of the process)	Mass Balance (Gas Stream)	$\dot{M}_{CombGas} = \dot{M}_{Ex}$	(3.14)
	Mass Balance (Product Stream)	$\dot{M}_{Prod,in} = \dot{M}_{Prod,out}$	(3.15)
	Enthalpy Balance (Gas Stream)	$q_{reac.} = \dot{M}_{Ex} \bullet h_{Ex} + q_{Heating} + q_{WH} + q_{Losses}$	(3.16)
	Enthalpy Balance (Product Stream)	$\dot{M}_{Prod,in} \bullet h_{Prod,in} + q_{Heating} = \dot{M}_{Prod,out} \bullet h_{Prod,out}$	(3.17)

It is to note that the parcel of the enthalpy allocated as useful energy ($q_{Heating}$) shall be constant for a single combustion-based process for all scenarios of operation (so to ensure that the allocated useful energy is the same for both the baseline and improved scenarios). In the scope of this work, it is intended as the produced material any solid, liquid or gaseous stream to which is necessary to be inputted a determinate quantity of enthalpy for the operation of the overall production process of a plant, which may not only be the produced good that is intended to result as an output of the combustion-based process (installed at any point from the upstream to the downstream of the whole plant production process) but also steam that is produced from freshwater in a steam boiler. It is to note that by a reason of convenience it is performed a difference of notation between the enthalpy that is allocated to waste heat streams (q_{WH}) and the one corresponding to remaining enthalpy losses (q_{Losses}). In Table 3-8, generalist flowsheet representations encompassing the parameters associated to each stream are presented.

Table 3-8. Generalist flowsheet representation of a Combustion-based process considering the aforementioned parameters associate to each stream

<table>
<tr><th>Phenomenon</th><th>Flowsheet representation</th></tr>
<tr><td>Direct Allocation of Enthalpy</td><td>
</td></tr>
<tr><td>Indirect Allocation of Enthalpy</td><td>
</td></tr>
</table>

ii) Modelling of Water Recirculation and Water-using Processes

The types of water systems included in the concept of WEIS (constituted by a set of water-using processes and wastewater treatment units) are highly based on the performance of water recirculation [98]. In addition to the splitting and mixing operation regarded in Table 3-4, the phenomena of heating and cooling must also be accounted in the case of this type of water system, corresponding to the input of hot and cold utilities in determinate points of the system. The general mass and enthalpy equations referent to water recirculation and water-using units, heating and cooling unit operations encompassed in a water system are presented in Table 3-9.

Table 3-9. Mass and enthalpy balance for a water system

Phenomenon		Equation	
		Water recirculation	
Global	Mass balance	$\dot{M}_{FW} = \dot{M}_{DW} + \dot{M}_{Sludge}$	(3.18)
	Enthalpy balance	$\dot{M}_{FW} \cdot h_{FW} + q_{Heating} + q_{WWT} = \dot{M}_{DW} \cdot h_{DW} + \dot{M}_{Sludge} \cdot h_{Sludge} + q_{Cooling}$	(3.19)
Splitting	Mass balance	$\dot{M}_{W,i} = \sum_{j=1} \dot{M}_{W,j}$	(3.20)
	Enthalpy balance	$h_{W,i} = h_{W,j}$	(3.21)
Mixing	Mass balance	$\sum_{j=1} \dot{M}_{W,j} = \dot{M}_{W,i}$	(3.22)

	Enthalpy balance	$\sum_{j=1} \dot{M}_{W,j} \cdot h_{W,j} = \dot{M}_{W,i} \cdot h_{W,i}$	(3.23)
Heating	Mass balance	$\dot{M}_{W,in} = \dot{M}_{W,out}$	(3.24)
	Enthalpy balance	$\dot{M}_{W,in} \cdot h_{W,in} + q_{Heater} = \dot{M}_{W,out} \cdot h_{W,out}$	(3.25)
Cooling	Mass balance	$\dot{M}_{W,in} = \dot{M}_{W,out}$	(3.26)
	Enthalpy balance	$\dot{M}_{W,in} \cdot h_{W,in} = \dot{M}_{W,out} \cdot h_{W,out} + q_{Cooler}$	(3.27)
Water-using Process			
Mass Balance (Water)		$\dot{M}_{W,in} = \dot{M}_{W,out}$	(3.28)
Mass Balance (Contaminant)		$\dot{M}_{W,in} \cdot C_{W,in} + \dot{M}_{cont.} = \dot{M}_{W,out} \cdot C_{W,out}$	(3.29)
Enthalpy Balance		$\dot{M}_{W,in} \cdot h_{W,in} + q_{WP} = \dot{M}_{W,out} \cdot h_{W,out}$	(3.30)

In the case of water-using processes, while an enthalpy allocation term (q_{WP}) is generically considered in the formulation of the enthalpy balance (which is positive in the case of heating and negative in the case of cooling), the majority of the cases approached in literature for Combined Water and Energy Integration generally consider that the passage of water stream through these processes is performed adiabatically (and as such this term is null).

3.2.2. Modelling of Heat Recovery Technologies

The phenomenon of heat transfer is the fundamental pillar of heat recovery technologies. Such phenomenon has different implications whether being analysed in a basis of steady-state operation or in transient mode. While the most standard equipment such heat exchangers being possible to be modelled according to its steady-state operation, thermal energy storage equipment must be analysed in terms of the occurrence of heat transfer in a transient mode.

i) Modelling of Heat Exchangers

The heat exchangers included in a Water and Energy Integration System may be economisers (the hot stream is a hot gas and the cold stream is water), air-preheaters (the hot stream is exhaust gas and the cold stream is air) and heat recovery steam generation units such as the one included in thermodynamic cycles, in which the hot stream is exhaust gas and the cold stream is a liquid). While the former two occur with both hot and cold fluids in the same phase, the latter involves phase transfer from liquid to vapour of the cold stream. In Table 3-10, the equations representing the whole phenomena occurring in heat exchangers are presented.

Table 3-10. General Mass and Enthalpy Balances and Heat Transfer equations for Heat Exchangers

Phenomenon	Equation	
Hot Fluid Balances		
Mass Balance	$\dot{M}_{Hot,in} = \dot{M}_{Hot,out}$	(3.31)
Enthalpy Balance	$\dot{M}_{Hot,in} \cdot h_{Hot,in} = \dot{M}_{Hot,out} \cdot h_{Hot,out} + q_{HT}$	(3.32)

Cold Fluid Balances			
Mass Balance		$\dot{M}_{Cold,in} = \dot{M}_{Cold,out}$	(3.33)
Enthalpy Balance		$\dot{M}_{Cold,in} \cdot h_{Cold,in} + eff_{HT} \cdot q_{HT} = \dot{M}_{Cold,out} \cdot h_{Cold,out}$	(3.34)
Heat Transfer			
Heat Transfer between two fluid streams		$q_{HT} = U \cdot A \cdot \Delta T_{med}$	(3.35)
	Co-current	$\Delta T_{med} = \left((T_{Hot,in} - T_{Cold,out}) \cdot (T_{Hot,out} - T_{Cold,in}) \cdot \left(\frac{(T_{Hot,in} - T_{Cold,out}) + (T_{Hot,out} - T_{Cold,in})}{2} \right) \right)^{1/3}$	(3.36)
	Counter-current	$\Delta T_{med} = \left((T_{Hot,in} - T_{Cold,in}) \cdot (T_{Hot,out} - T_{Cold,out}) \cdot \left(\frac{(T_{Hot,in} - T_{Cold,in}) + (T_{Hot,out} - T_{Cold,out})}{2} \right) \right)^{1/3}$	(3.37)
Evaporation	**Inlet to Saturated Liquid**	$q_L = \dot{M} \cdot (h_{vap,L} - h_{in})$	(3.38)
	Phase change	$q_{vap} = \dot{M} \cdot (h_{vap,V} - h_{vap,L})$	(3.39)
	Saturated Vapour to Outlet	$q_V = \dot{M} \cdot (h_{out} - h_{vap,V})$	(3.40)

The equations for the determination of mean temperature difference (equations (3.36) and (3.37)) are formulated according to the respective forms using Chen's approximation [372] of the logarithmic mean temperature difference, which is set to be the form used to compute such measure in the models furtherly presented. In the case of the enthalpy balance equation formulated for the cold stream (equation (3.34)), a heat transfer efficiency parcel (eff_{HT}) is considered (ensuring that the enthalpy that is withdrawn from the hot stream is either allocated to the cold stream or as heat losses).

ii) Modelling of Latent Thermal Energy Storage

The set to be developed models for thermal energy storage essentially subsist on the setup of time-depending heat transfer variables and equations (as demanded by the requirement to assess the variation of specific enthalpy/ temperature along time by the supply of enthalpy from an external heat source). In a general manner, heat transfer within a thermal energy storage unit is proceeded by the enthalpy withdrawal/ supply from/ to a heat transfer fluid (HTF) to the mass of storage material within a vessel, with these phenomena corresponding respectively to the charging and discharging of enthalpy into/ from the storage material. While the mass/ enthalpy balances on the side of the heat transfer fluid are generally formulated by the same set of equations for a heat exchanger (with the only exception of being associated to a time-variating heat duty), for the storage material-side enthalpy balances are formulated taking into account a static mass and a variating specific enthalpy/ temperature. The heat transfer equations correspond to equations that account for the phenomenon of heat conduction and natural convection. In Table 3-11, the equations that characterize a TES unit (modelled according to the case of PCM-TES type of technologies) are presented.

Table 3-11. Equations for the Variation between Temperature, Specific Enthalpy and Stored Enthalpy

Phenomenon	Equation	
	Heat Transfer Fluid	
Mass Balance	$\dot{M}_{HTF,in} = \dot{M}_{HTF,out}$	(3.41)
Enthalpy Balance	$\dot{M}_{HTF,in} \cdot h_{HTF,in} = \dot{M}_{HTF,out} \cdot h_{HTF,out} + q_{HT}$	(3.42)
	Phase change material	
Enthalpy Balance	$H_{PCM} = M_{PCM} \cdot h_{PCM}$	(3.43)
Heat Transfer	$\frac{dH_{PCM}}{dt} = q_{HT}$	(3.44)
	$\frac{1}{r^n} \cdot \frac{d}{dr}\left(r^n \cdot k \cdot \frac{dT_{PCM}}{dr}\right) = \rho \cdot C_p \cdot \frac{dT_{PCM}}{dt}$	(3.45)

It is to note that the for the case of the PCM-side heat transfer equations only the conduction equation is presented. Such is attributed to the current state of development of the ThermWatt Modelica library thermal energy storage component models, in which the convective heat transfer phenomenon is neglected. The equation enunciated for heat conduction (equation (3.45)) results of an adaptation of the generic heat conduction equation [373] in which the energy-generating term is null. This equation is also formulated for any geometry, having to be adapted in model development for the case of each geometry in specific ($n = 0$ for plane geometry, $n = 1$ for cylindrical geometry and $n = 2$ for spherical geometry). Moreover, the formulation of the presented equation the transferred enthalpy term (q_{HT}) is positive for charging and negative for discharging.

The relation between the specific enthalpy and temperature of the PCM are established in literature by two different methods:

- Specific enthalpy method, in which three relations between specific enthalpy and temperature are established for respectively the solid phase, phase change and liquid phase;
- Apparent specific heat capacity method, in which a single relation equation is established between these two variables through an adaptation of equation (3.6), in which the specific heat capacity ($C_{P,PCM}$) is the one to change according to different values of specific enthalpy/ temperature (it is set as the respective theoretical values for the solid and liquid phases and for the phase change it takes considerably high values to account for the corresponding latent heat and small variation of temperature).

Both these methods are set to be used for the development of the equipment-level models, with a single one being selected for each case according to the convenience of the running of the simulation and optimisation models.

3.2.3. Modelling of Heat-Driven Wastewater Treatment Units

The development of heat-driven wastewater treatment (HDWWT) units such as the ones approached in chapter 2 subsist on the gathering of equations that express the phenomenon of heat transfer between a determinate heat source stream and the water/ wastewater stream at the inlet of an effect constituent of a HDWWT unit. In the formulation of the equations that characterize these units, it is necessary to ensure that the quantity of generated steam in a constituent effect (and thus the quantity of treated water) depends on allocated enthalpy from the heat source stream (or rather from the vapour stream that results from a previous effect). The mass/ enthalpy balances and heat transfer equations characterizing a generic HDWWT unit are presented in Table 3-12.

Table 3-12. General mass and enthalpy balance equations for HDWWT technologies

Phenomenon	Equation	
Wastewater/ Treated water Side (Overall)		
Mass Balance (Water)	$\dot{M}_{WW} = \dot{M}_{TW} + \dot{M}_{Sludge}$	(3.46)
Mass Balance (Contaminant)	$\dot{M}_{WW} \cdot C_{WW} = \dot{M}_{TW} \cdot C_{TW} + \dot{M}_{Sludge} \cdot C_{Sludge}$	(3.47)
Enthalpy Balance	$\dot{M}_{WW} \cdot h_{WW} + q_{WWT} = \dot{M}_{TW} \cdot h_{TW} + \dot{M}_{Sludge} \cdot h_{Sludge}$	(3.48)
Vapour Side (Single Unit)		
Mass Balance (Water)	$\dot{M}_{WW,Unit} = \dot{M}_{V,Unit} + \dot{M}_{Sludge,Unit}$	(3.49)
	$\frac{\dot{M}_{V,Unit}}{\dot{M}_{WW,Unit}} = \frac{h_{out} - h_L}{h_V - h_L}$	(3.50)
Mass Balance (Contaminant)	$\dot{M}_{WW,Unit} \cdot C_{WW,Unit} = \dot{M}_{V,Unit} \cdot C_{V,Unit} + \dot{M}_{Sludge,Unit} \cdot C_{Sludge,Unit}$	(3.51)
Enthalpy Balance	$\dot{M}_{WW,Unit} \cdot h_{WW,Unit} + q_{WWT,Unit} = \dot{M}_{V,Unit} \cdot h_{final,Unit} + \dot{M}_{Sludge,Unit} \cdot h_{Sludge,Unit}$	(3.52)
Heat Source Stream Side		
Mass Balance	$\dot{M}_{HS,in} = \dot{M}_{HS,out}$	(3.53)
Enthalpy Balance	$\dot{M}_{HS,in} \cdot h_{HS,in} = \dot{M}_{HS,out} \cdot h_{HS,out} + q_{WWT}$	(3.54)
Vapour Stream (from a previous effect)		
Mass Balance	$\dot{M}_{V,in} = \dot{M}_{TW,out}$	(3.55)
Enthalpy Balance	$\dot{M}_{HS,in} \cdot h_{V,in} = \dot{M}_{TW,out} \cdot h_L + q_{WWT}$	(3.56)
Heat Transfer		
	$q_{WWT} - \dot{M}_{WW} \cdot (h_L - h_{in}) = U \cdot A \cdot \Delta T_{med}$	(3.57)
	$\Delta T_{med} = \left(\left(T_{HS,in} - T_{W,out}\right) \cdot \left(T_{HS,out} - T_{W,in}\right) \cdot \left(\frac{\left(T_{HS,in} - T_{W,out}\right) + \left(T_{HS,out} - T_{W,in}\right)}{2} \right) \right)^{1/3}$	(3.58)

For the convenience of the presentation of the formulated equations a corresponding set of equations for vapour stream are enunciated based on the same set of equations for wastewater/ treated water side. While the former equation set is applied to single units of a specific HDWWT technology (such as the effects of Multi-effect distillation (MED) and the stages of Multi-stage flash distillation (MSFD)), the latter corresponds to overall mass/ enthalpy balances for the whole HDWWT unit. For the case of the heat source stream, a derivative separated set of equations is enunciated for the vapour stream from a previous effect, taking into account that:

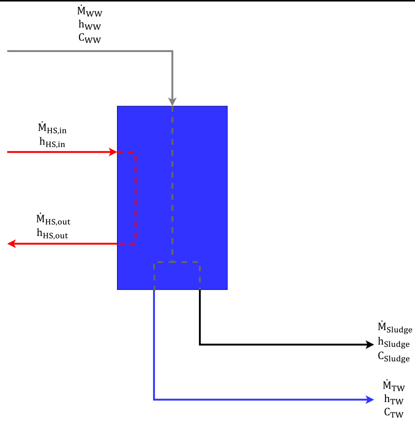
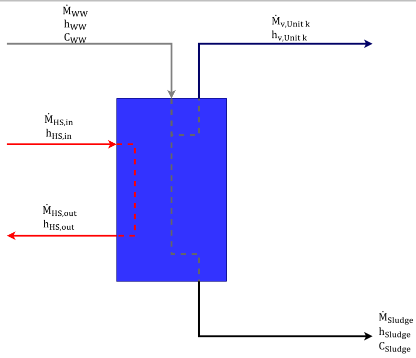
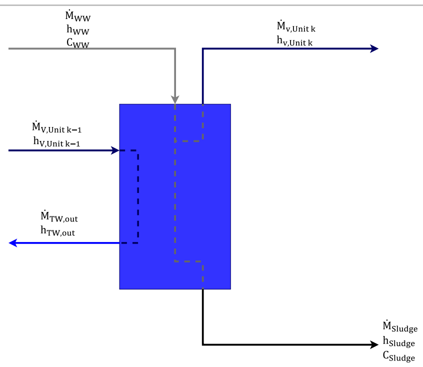
- For a certain sub-unit of the whole HDWWT unit (such as the first effect of MED and the brine heater of MSFD) the hot stream is an external heat source stream (such as a gas stream resulting as a waste heat stream from a combustion-based process);

- For the remaining sub-units, the hot stream is the vapour stream from a previous sub-unit, which is condensed on the present sub-unit (such as the second-to-last effects in MED and the stages in MSFD).

The allocated enthalpy terms (q_{WWT} and $q_{WWT,Unit}$) are respectively formulated for the overall mass/ enthalpy balances (q_{WWT}) (this is also the enthalpy withdrawn from the external heat source in the division such stream is involved) and for each division ($q_{WWT,Unit}$). The heat transfer equations (3.57) and (3.58) result as an adaption of equations (3.35) and (3.36).

In Table 3-13, it is presented by a reason of convenience an association of the aforementioned stream parameters to an overall HDWWT unit and each constituting sub-unit, in the form of flowsheet representations.

Table 3-13. Generalist flowsheet representations relative to an overall HDWWT unit and each constituting sub-unit

Unit	Flowsheet representation
Overall HDWWT Unit	
Single Unit (External heat source stream)	
Single Unit (Vapour from previous unit used as the heat source stream)	

3.2.4. Modelling of Wastewater-to-energy Technologies

For the purpose of energy recovery from discharge water streams resulting from water system, several technologies may be implemented for different ends at the level of fuel production, as approached in section 2.4. The equations that represent the conversion of water and wastewater quantities into additional fuel quantities must establish a relation between the flow rate of sludge (such as the on resulting from wastewater treatment) and the flow rate of produced fuel. Moreover, the formulated must also account for the quantity of thermal or electric energy that must be allocated to wastewater-to-energy units for the purpose of producing additional fuel. The equations that express generic mass and energy balances in wastewater-to-energy units are presented in Table 3-14.

Table 3-14. General mass and energy balance for wastewater-to-energy units

Phenomenon	Equations	
Mass Balance	$\dot{M}_{Sludge} \cdot eff_{WWtE} = \dot{M}_{additional\ fuel}$	(3.59)
Energy Balance	$q_{required} \cdot eff_{WWtE} = Pot_{supply} \cdot eff_{conversion}$	(3.60)

In the formulation of the equations presented in Table 3-14, terms for mass and energy conversion are considered, namely the conversion of the inlet water/ sludge stream to additional fuel (eff_{WWtE}) and the conversion of the inlet energy source to the effectively useful energy for the occurrence of conversion reaction phenomena ($eff_{conversion}$), which is for instance the case of the allocation of electricity to an Electrolysis unit to be supplied for the occurrence of the overall reaction of water splitting. In the prospect of this formulation, the variable conversion of the inlet water/ sludge into fuel and the inlet energy source into useful energy is accounted in a generic form.

3.3. Model Development

The development of component-level simulation models approached in this work includes the modelling of each one of the unit operations that characterize a Water and Energy Integration System (WEIS) and the respective interconnections (stream recirculation and allocation of energy vectors). A set of auxiliary components (not representing physically existing equipment) are also necessary to model specific requirements. The model development procedure takes into account the most generic governing equations presented in section 3.2 adapted to each case in specific, namely to each industrial process and to-be-considered technology. While this procedure is primarily performed for the purpose of the development of simulation models, the optimisation models set to be developed on the scope of this work take into account the same set of equations, physical phenomena consideration-related simplifications and assumptions (performed for the purpose of the increase of the robustness of these models). All the equipment-level and system-level simulation models are set to be part of the ThermWatt

Modelica library, which is part of the overall ThermWatt computational tool. The selection of the Modelica language and the OpenModelica package (in particular) for the development of the main module of the overall ThermWatt tool (which is the simulation tool) is attributed to characteristics of the modelling language [374] and the package [370]:

- **Acausal and declarative modelling**: inexistence of the explicit reference to the order in which equations are solved;
- **Transparency of the developed code**: possibility to write the equations in the same form these are written in paper;
- **Encapsulation and modularity of the modelling procedure**: separation between elementary models (roughly define by a set of equations and variables) and aggregate models (defined by the interconnection between several elementary models);
- **Inheritance of model development**: opportunity to further develop more complex from more simple models through the addition of equations and variables of interest for a determinate case;
- **Multi-physics modelling**: possibility to model several types of physical phenomena;
- **Reusability of models**: continuous development of models, through the creation of gradually more updated versions of these models (the previous version of the model serving as a reference for the more updated version);
- **Opportunity to couple with other software packages**: possibility to allocate results from a model developed in a separate package (such as in the Python language) to a Modelica model (which is the case of the OpenModelica Python API).

Software architecture of the ThermWatt Modelica Library

The component models (which are simulation models for all the single unit operations of interest) are allocated to different packages of the ThermWatt Modelica library, typically according to the different industrial sectors these are inserted. Nonetheless, component models that exist transversally to all sectors of the manufacturing industry existing within a package designated as *Transversal* (which is the case of boilers). In the case of specific technologies, such as heat recovery, thermal storage and wastewater treatment, these exist within proper packages. As the majority of the component models in the context of this work are new developments (these are not present in any available library developed before using the Modelica language), each one of the mentioned unit operations models will be validated with real plant measured data. In Table 3-15, the packages that were developed under this work and included in the ThermWatt library are characterized.

Table 3-15. Characterization of packages of the ThermWatt Modelica library

Package	Characterization
General	It contains basic models for fluid flow (for instance, source, discharge and passage) associated to several fluid media; It is divided in sub-packages each one corresponding to different media (each sub-package

	roughly contains versions for the same type of models): • Gases (itself divided in Natural Gas, HENG, Air and Exhaust); • Water; • Organic Fluids.
Main Packages	
Ceramic	It contains models for the combustion-based thermal processes present in a ceramic plant.
Heat Exchangers *(HeatExchangers)*	It contains models for several types of heat exchangers, such as: • Water-gas heat exchanger (Economiser); • Air-gas heat exchanger (Air-preheater).
Cycles	It contains models for the equipment present in thermodynamic cycles (sub-packages exist for each type of cycle). At the date of the development of this work, only the models referent to the Organic Rankine Cycle (ORC) have been developed: • Heat recovery steam generator (HRSG) unit; • Vapour turbine; • Electricity generator; • Regenerator; • Condenser; • Centrifugal Pump (Main cycle); • Centrifugal Pump (Cooling water cycle); • Cooling Tower (Cooling water cycle).
Storage	It contains models for thermal energy storage units. At the date of the development of this work, only latent TES technology models have been fully developed: • PCM-filled tank (water as heat transfer fluid); • PCM-based heat exchanger.
Wastewater Treatment	It contains models for water system containing wastewater treatment units. It includes all the system-level components that characterize water flow (a part of these components results from an adaption of the same models present in the General package). It mainly contains the model for the generic water-using process and wastewater treatment technologies. At the time of development of this work, only heat-driven wastewater treatment unit models have been developed, with the only considered in this case being Multi-effect distillation: • First Effect (hot gas stream as heat transfer fluid); • Second Effect; • Condenser.
Wastewater-to-energy *(WWtE)*	It contains model for technologies for energy recovery from wastewater. At the time of the development of this work, only an Electrolysis unit model had been developed.
Base Classes *(BaseClasses)*	It contains code for basic models that are furtherly adapted (such as the basic occurring phenomena in pipes/ ducts).
Structural Packages	
Media	It contains packages for each one of the fluid media necessary to consider, namely: • Water; • Natural gas; • Hydrogen-enriched natural gas; • Air; • Exhaust Gas; • Organic fluid NOVEC649.
Units	It contains packages for several units of measurements (which are used to define each constant, parameter and variable characterizing each model).
Icons	It contains models for the icons that visually appear on the canvas of the Modelica distribution environment (in this case, OpenModelica).

Choices	It contains packages for non-numerical options in several models.
Functions	It contains functions (input/ output correspondence) to be considered in several models.
Constants	It contains defined constants (namely material properties), which are conveniently used in each equipment-level model.

Moreover, the ThermWatt Modelica library has been developed based on the software structure inherent to existing Modelica libraries, namely in terms of package division and coding methods. Although the library mostly uses newly developed code, it adapts a part of the code of the open-source ThermoPower Library, namely for the majority of the components present in the *General* package and the remaining system-wide components, with this library serving as necessary and mandatory dependence of the ThermWatt library.

In the context of the characterization of the referred models, it is generally performed a distinction between the following types of variables (based on the designations proper of the Modelica language):

- Parameters (which are independent variables and may be defined by the user);
- Variables (which are dependent variables and as such are calculated through the definition of the parameters and the solving of the governing equations).

In the context of the characterization of the status of the models in terms of innovation (in relation to existing models in other Modelica libraries), the following distinction is performed:

- New (which are models that have been developed in the context of the ThermWatt library, whose Modelica code has been created from root);
- Existing (which are models that exist in other Modelica libraries and have been adapted to be part of the ThermWatt library, with few alterations on the base Modelica code);

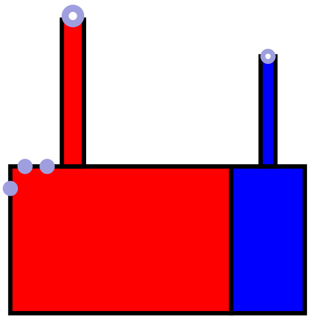
3.3.1. Models for Baseline processes and System-level components

The generality of the industrial system approached in this work contain combustion-based thermal processes, water-using processes, water heaters, water coolers and gas/ water flow components. All these processes/ unit operations must be modelled for all baseline and improved scenarios to be simulated/ optimised.

i) Combustion-based and Water-using processes

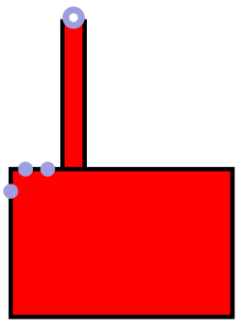
The main packages of ThermWatt contain a set of combustion-based and water-using processes, which are also the baseline of the previously presented Water and Energy Integration System (WEIS) concept. In Tables 3.16 and Table 3-17, the baseline industrial processes models that make part of the ThermWatt Modelica library are characterized. All the characterized combustion-based processes are equipment installed in the ceramic industry (a sector whose significant energy intensity is attributed to the functioning of these processes and in which the case-studies approached in the further chapters of this work are inserted on).

Table 3-16. Characterization of combustion-based and water-using process models (Continuous-type processes)

<table>
<tr><th colspan="3">Tunnel kiln</th></tr>
<tr><th>Category within the library</th><th colspan="2">New</th></tr>
<tr><td></td><td colspan="2">It is a model of tunnel kiln (installed in the firing step in whole the ceramic production process);
It considers the following sets of streams:
• Inlet fuel (HENG)/ Inlet combustion air/ Outlet exhaust gases;
• Inlet cooling air/ outlet hot air;
• Inlet ceramic material/ Outlet ceramic material;
The inlet ports correspond to each inlet stream identified above, with an additional port for recirculated air (in non-heat recovery scenarios an air source with near-zero flow rate is interconnected to it);
It considers the mandatory input of the following parameters:
• Initial mass flow rate of fuel;
• Initial air-to-fuel ratio;
• Temperature of fuel;
• Initial temperature of combustion air;
• Mass flow rate of material;
• Inlet temperature of material;
• Outlet temperature of material;
• Mass flow rate of cooling air;
• Inlet temperature of cooling air;
• Outlet temperature of hot air;
• Total heat losses;
The model is described by the same set of equations presented below, overall resulting of an adaption of the equations present in section 3.2.1 – i);
It assumes that the parcels for the enthalpy to be allocated to the ceramic material, cooling/ hot air stream and to heat losses are constant (not variating according to the different conditions of the inlet fuel and combustion air).</td></tr>
<tr><td rowspan="2">Combustion Chamber</td><td>$\dot{M}_{Fuel} + \dot{M}_{C.Air} = \dot{M}_{Ex}$</td><td>(3.61)</td></tr>
<tr><td>$\dot{M}_{Fuel} \bullet (h_{Fuel} + LHV) + \dot{M}_{Air} \bullet h_{Air} = \dot{M}_{Ex} \bullet h_{CombGas}$</td><td>(3.62)</td></tr>
<tr><td rowspan="4">Heating Zone</td><td>$\dot{M}_{CombGas} = \dot{M}_{ExGas}$</td><td>(3.63)</td></tr>
<tr><td>$\dot{M}_{Ceramic,in} = \dot{M}_{Ceramic,out}$</td><td>(3.64)</td></tr>
<tr><td>$\dot{M}_{CombGas} \bullet h_{CombGas} = \dot{M}_{Ex} \bullet h_{Ex} + q_{Heating} + q_{Cooling} + q_{Losses}$</td><td>(3.65)</td></tr>
<tr><td>$\dot{M}_{Ceramic,in} \bullet h_{Ceramic,in} + q_{Heating} = \dot{M}_{Ceramic,out} \bullet h_{Ceramic,out}$</td><td>(3.66)</td></tr>
<tr><td rowspan="4">Cooling Zone</td><td>$\dot{M}_{Cool.Air,in} = \dot{M}_{Cool.Air,out}$</td><td>(3.67)</td></tr>
<tr><td>$\dot{M}_{Ceramic,in} = \dot{M}_{Ceramic,out}$</td><td>(3.68)</td></tr>
<tr><td>$\dot{M}_{Cool.Air,in} \bullet h_{Cool.Air,in} + q_{Cooling} = \dot{M}_{Cool.Air,out} \bullet h_{Cool.Air,out}$</td><td>(3.69)</td></tr>
<tr><td>$\dot{M}_{Ceramic,in} \bullet h_{Ceramic,in} = \dot{M}_{Ceramic,out} \bullet h_{Ceramic,out} + q_{Cooling}$</td><td>(3.70)</td></tr>
<tr><td rowspan="4">Overall</td><td>$\dot{M}_{Fuel_{Baseline}} \bullet LHV_{NG} = \dot{M}_{Fuel} \bullet LHV_{Fuel} + q_{additional,kiln}$</td><td>(3.71)</td></tr>
<tr><td>$q_{additional,kiln} = \dot{M}_{C.Air} \bullet \left(h_{C.Air} - h_{C.Air,Baseline}\right)$</td><td>(3.72)</td></tr>
<tr><td>$LHV_{Fuel} = LHV_{NG} \bullet Y_{NG} + LHV_{H_2} \bullet Y_{H_2}$</td><td>(3.73)</td></tr>
<tr><td>$AF_{Fuel} = AF_{NG} \bullet \frac{LHV_{Fuel}}{LHV_{NG}}$</td><td>(3.74)</td></tr>
<tr><th colspan="3">Water-using Process</th></tr>
<tr><th>Category within the library</th><th colspan="2">New</th></tr>
</table>

	It is a model for a generic water-using process, in which an inlet water stream is set to remove a certain quantity of contaminants, leaving the resulting stream as wastewater; The model only considers as necessary parameter the mass flow rate of each contaminant to be removed; The model is described by the same set of equations presented below, overall resulting of an adaption of the equations present in section 3.2.1 – ii). It assumes the inexistence of the contribution of the inlet contaminant stream on the enthalpy balance, owing to the lower order of magnitude of the mass flow rate of contaminant in relation to water (which is verified in most real-life case-studies). It also assumes the inexistence of variation on the stream physical properties due to the mixture between water and contaminants.
$\dot{M}_{W,in} = \dot{M}_{W,out}$	(3.75)
$\dot{M}_{W,in} \cdot C_{W,in} + \dot{M}_{cont.} = \dot{M}_{W,out} \cdot C_{W,out}$	(3.76)
$\dot{M}_{W,in} \cdot h_{W,in} = \dot{M}_{W,out} \cdot h_{W,out}$	(3.77)

Table 3-17. Characterization of combustion-based and water-using process models (Batch-type processes)

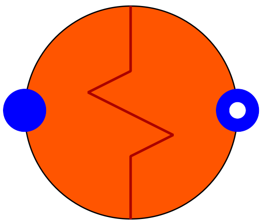
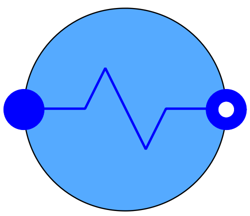
Intermittent Kiln		
Category within the library	New	
	It is a model of intermittent kiln (typically installed in ceramic industry plants for the firing step); It considers the following sets of streams: • Inlet fuel (HENG)/ Inlet combustion air/ Outlet exhaust gases; • Inlet ceramic material/ Outlet ceramic material; The inlet ports correspond to each inlet stream identified above, with an additional port for recirculated air (in non-heat recovery scenarios an air source with near-zero flow rate is interconnected to it); It considers as necessary parameters: • Initial mass flow rate of fuel; • Initial air-to-fuel ratio; • Temperature of fuel; • Initial temperature of combustion air; • Mass flow rate of material; • Inlet temperature of material; • Outlet temperature of material; • Total heat losses; The model is described by the same set of equations presented below, overall resulting of an adaption of the equations present in section 3.2.1 – i); It assumes that the parcels for the enthalpy to be allocated to the ceramic material and to heat losses are constant (not variating according to the different conditions of the inlet fuel and combustion air).	
Combustion Chamber	$\dot{M}_{Fuel} + \dot{M}_{C.Air} = \dot{M}_{Ex}$	(3.78)
	$\dot{M}_{Fuel} \bullet (h_{Fuel} + LHV) + \dot{M}_{Air} \bullet h_{Air} = \dot{M}_{Ex} \bullet h_{CombGas}$	(3.79)
Heating Zone	$\dot{M}_{CombGas} = \dot{M}_{Ex}$	(3.80)
	$\dot{M}_{Ceramic,in} = \dot{M}_{Ceramic,out}$	(3.81)
	$\dot{M}_{CombGas} \bullet h_{CombGas} = \dot{M}_{Ex} \bullet h_{Ex} + q_{Heating} + q_{Losses}$	(3.82)
	$\dot{M}_{Ceramic,in} \bullet h_{Ceramic,in} + q_{Heating} = \dot{M}_{Ceramic,out} \bullet h_{Ceramic,out}$	(3.83)
Overall	$\dot{M}_{Fuel_{Baseline}} \bullet LHV_{NG} = \dot{M}_{Fuel} \bullet LHV_{Fuel} + q_{additional}$	(3.84)

$$q_{additional,kiln} = \dot{M}_{Comb.Air} \bullet \left(h_{C.Air} - h_{C.Air,Baseline}\right)$$	(3.85)
$$LHV_{Fuel} = LHV_{NG} \bullet Y_{NG} + LHV_{H_2} \bullet Y_{H_2}$$	(3.86)
$$AF_{Fuel} = AF_{NG} \bullet \frac{LHV_{Fuel}}{LHV_{NG}}$$	(3.87)

ii) Water System energy-using components

The water system encompassed in the WEIS concept contain a determinate number of hot utility-using units (heaters) and cold utility-using ones (coolers) that make of the water system. In Table 3-18, the water system heaters and coolers models that make part of the ThermWatt Modelica library are characterized.

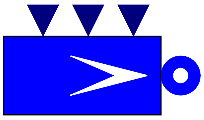
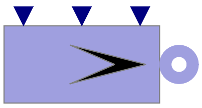
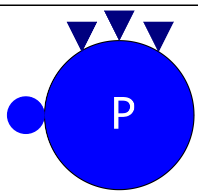
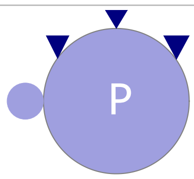
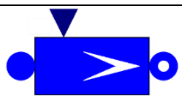
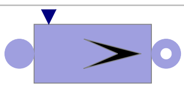
Table 3-18. Characterization of water system heater and cooler models

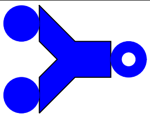
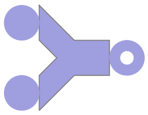
Heater		
Category within the library	New	
	It is a heat exchanger set to be installed in a water system for the heating of a water stream to a determinate objective temperature; It considers the input of a determinate quantity of hot utility, whose associated enthalpy is calculated according to the conditions of the inlet water stream; It considers as necessary parameters: • Objective outlet temperature of the water stream ($T_{W,out}$); • Efficiency associated to water heating by the hot utility (eff_{Heater}); It does not consider an inlet port for the hot stream (hot utility); The model is generally described by the equations presented above, resulting as an adaption of the mass and enthalpy balance equations presented in Table 3-10.	
$$\dot{M}_{W,in} = \dot{M}_{W,out}$$		(3.88)
$$\dot{M}_{W,in} \bullet C_{W,in} = \dot{M}_{W,out} \bullet C_{W,out}$$		(3.89)
$$\dot{M}_{W,in} \bullet h_{W,in} + q_{Hot\,Ut.} \bullet eff_{Heater} = \dot{M}_{W,out} \bullet h_{W,out}$$		(3.90)
Cooler		
Category within the library	New	
	It is a heat exchanger set to be installed in a water system for the cooling of a water stream to a determinate objective temperature; It considers the input of a determinate quantity of cold utility, whose associated enthalpy is calculated according to the conditions of the inlet water stream; It considers as necessary parameters: • Objective outlet temperature of the water stream ($T_{W,out}$); • Efficiency associated to the cold utility ($eff_{Cool.Ut.}$); It does not consider an inlet port for the cold stream (cold utility); The model is generally described by the equations presented above, resulting as an adaption of the mass and enthalpy balance equations presented in Table 3-10.	
$$\dot{M}_{W,in} = \dot{M}_{W,out}$$		(3.91)
$$\dot{M}_{W,in} \bullet C_{W,in} = \dot{M}_{W,out} \bullet C_{W,out}$$		(3.92)
$$\dot{M}_{W,in} \bullet h_{W,in} = \dot{M}_{W,out} \bullet h_{W,out} + q_{Cool.Ut.} \bullet eff_{Cool.Ut.}$$		(3.93)

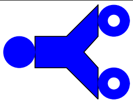
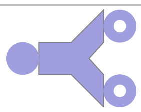
iii) System-wide Components

The conceptualization and implementation of WEIS require the project of the installation of liquid pipes, gas ducts and mixing/ splitting units that serve as interconnections between several unit operations and as such allow stream recirculation. In Table 3-19, the system-wide component models that make part of the ThermWatt Modelica library are characterized.

Table 3-19. Characterization of overall system component models

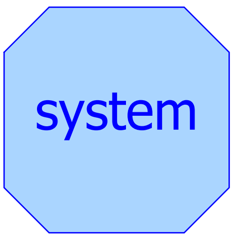
Source	
Category within the library	Existing Minor modifications performed from corresponding ThermoPower library models for user-friendliness purposes (change of units of parameters)
 	These are fluid stream source components, in which following necessary parameters are defined: • Mass flow rate; • Temperature; • Pressure; Mass fraction associated to each component of a gas (only for the gas source, depends on the number of components of each gas); Additional inlet ports (the arrows on the top of the figures) exist for variating mass flow rates, temperature and gas composition (in the case of the gas).
Sink	
Category within the library	Existing Minor modifications performed from corresponding ThermoPower library models for user-friendliness purposes (change of units of parameters)
 	These are fluid stream sink components, in which the outlet pressure may be defined.
Passage	
Category within the library	Existing Minor modifications performed from corresponding ThermoPower library models for user-friendliness purposes (change of units of parameters)
 	These are fluid passage sink components, in which the associated mass flow rate may be defined; These are commonly applied in the case of stream splitting, in which these define the mass flow rate of one of the separated streams; An additional inlet port (the arrow at the top of the figures) exists for variating mass flow rates.
Mixer	
Category within the library	Existing

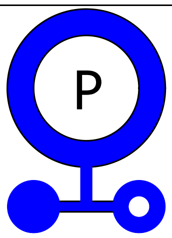
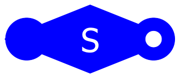
 	These are fluid stream mixing components, which consider the input of two streams of the same medium; The mass and enthalpy balance equations are described by equations (3.94) – (3.96); An additional mixer component exists for the mixing of two gases of different media (air and flue gas), described by the same set of equations.	
	$\dot{M}_{in,1} + \dot{M}_{in,2} = \dot{M}_{out}$	(3.94)
	$\dot{M}_{in,1} \bullet h_{in,1} + \dot{M}_{in,2} \bullet h_{in,2} = \dot{M}_{out} \bullet h_{out}$	(3.95)
Water component only	$\dot{M}_{in,1} \bullet C_{in,1} + \dot{M}_{in,2} \bullet C_{in,2} = \dot{M}_{out} \bullet C_{out}$	(3.96)

Splitter		
Category within the library	Existing	
 	These are fluid stream splitting components, separating a stream in two; The mass flow rates of each separate stream may be defined by the passage components.	
	$\dot{M}_{in} = \dot{M}_{out,1} + \dot{M}_{out,2}$	(3.97)
	$h_{in} = h_{out,1}$	(3.98)
	$h_{in} = h_{out,2}$	(3.99)
Water component only	$C_{in} = C_{out,1}$	(3.100)
	$C_{in} = C_{out,2}$	(3.101)

In addition to the previously presented components, a set of models that serve for the setup of the simulation process have been developed, not representing any particular equipment of the WEIS or rather not being directly involved in the physical phenomena modelling (for instance, equipment that is set to serve for process control purposes). In Table 3-20, the models of the aforementioned category are characterized.

Table 3-20. Characterization of miscellaneous overall system component models

System Definition	
Category within the library	Existing
	It is a component that must be inserted in each simulation model in particular, so to define basic but fundamental setup parameters for the simulation; For instance, the following parameters are set to be defined: Mode operation (Steady-state for steady-state based simulation or Fixed-state for the case of dynamic simulation); Flow reversal operation (Existence or non-existence of flow reversal); Ambient conditions (ambient pressure, wet-bulb ambient temperature and dry-bulb ambient temperature).
Expansion Tank	
Category within the library	Existing

	It is a component set to be included in-between the outlet from one unit operation and the inlet of another to define the stream pressure (the simulation runs so to respect that specific pressure constraint); It is essentially set to be installed in closed circuit systems (for instance, thermodynamic cycles).
Stream Sensors	
Category within the library	Existing
 	These are components that are set to be included in-between the outlet from one unit operation and the inlet of another to measure the parameters associated to involved stream (mass flow rate, temperature, specific enthalpy and pressure).

3.3.2. Heat Recovery Technologies

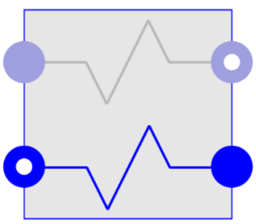
The ThermWatt library contains a set of heat recovery technologies that make part of three of the main packages:

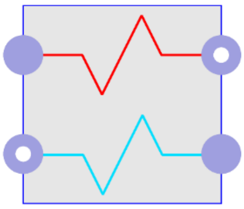
- Heat Exchangers (all models for heat exchangers set to be installed for pre-heating of a determinate stream at the inlet of an energy-using units);
- Cycles (all models that are part of thermodynamic cycles);
- Storage (all models for TES units or that are involved in auxiliary systems containing TES units).

i) Heat Exchangers

The heat exchanger models existing in the ThermWatt library are generally set for enthalpy withdrawal from a waste heat stream (generally an exhaust gas or hot air stream) to an air or water stream that is transported to an energy-using units (either a combustion-based process or a heater). In Table 3-21, the heat exchanger models of this category are characterized.

Table 3-21. Characterization of heat exchangers models

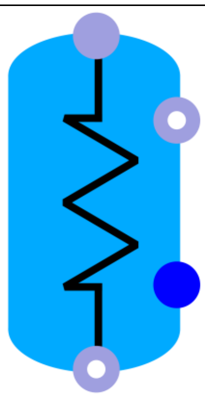
Water-gas heat exchanger (Economiser)		
Category within the library	New	
	It is a component that represent the water-gas heat exchanger technology operating in counter-current operation, in which the hot stream is an exhaust gas stream and the cold stream is a water stream; It considers as necessary parameters: • Overall heat transfer coefficient; • Heat transfer area or Temperature of the outlet water stream; The model is generally described by the equations presented below, resulting as an adaption of the equations presented in Table 3-10.	
Gas-side	$\dot{M}_{Gas,in} = \dot{M}_{Gas,out}$	(3.102)
	$\dot{M}_{Gas,in} \cdot h_{Gas,in} = \dot{M}_{Gas,out} \cdot h_{Gas,out} + q_{HT}$	(3.103)

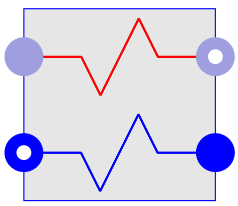
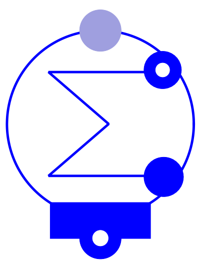
Water-side	$\dot{M}_{Cold,in} = \dot{M}_{Cold,out}$	(3.104)
	$\dot{M}_{Cold,in} \cdot C_{Cold,in} = \dot{M}_{Cold,out} \cdot C_{Cold,in}$	(3.105)
	$\dot{M}_{Cold,in} \cdot h_{Cold,in} + eff_{HT} \cdot q_{HT} = \dot{M}_{Cold,out} \cdot h_{Cold,out}$	(3.106)
Heat Transfer	$q_{HT} = U \cdot A \cdot \Delta T_{med}$	(3.107)
	$\Delta T_{med} = \left((T_{Hot,in} - T_{Cold,in}) \cdot (T_{Hot,out} - T_{Cold,out}) \cdot \left(\frac{(T_{Hot,in} - T_{Cold,in}) + (T_{Hot,out} - T_{Cold,out})}{2} \right) \right)^{1/3}$	(3.108)
Air-gas heat exchanger (Air preheater)		
Category within the library	New	
	It is a component that represent the air-gas heat exchanger technology operating in counter-current operation, in which the hot stream is an exhaust gas stream and the cold stream is an air stream; It considers as necessary parameters: • Overall heat transfer coefficient; • Heat transfer area or Temperature of the outlet air stream; The model is generally described by the equations presented below, resulting as an adaption of the equations presented in Table 3-10.	
Hot Gas-Side	$\dot{M}_{Hot,in} = \dot{M}_{Hot,out}$	(3.109)
	$\dot{M}_{Hot,in} \cdot h_{Hot,in} = \dot{M}_{Hot,out} \cdot h_{Hot,out} + q_{HT}$	(3.110)
Air-side	$\dot{M}_{Cold,in} = \dot{M}_{Cold,out}$	(3.111)
	$\dot{M}_{Cold,in} \cdot h_{Cold,in} + eff_{HT} \cdot q_{HT} = \dot{M}_{Cold,out} \cdot h_{Cold,out}$	(3.112)
Heat Transfer	$q_{HT} = U \cdot A \cdot \Delta T_{med}$	(3.113)
	$\Delta T_{med} = \left((T_{Hot,in} - T_{Cold,in}) \cdot (T_{Hot,out} - T_{Cold,out}) \cdot \left(\frac{(T_{Hot,in} - T_{Cold,in}) + (T_{Hot,out} - T_{Cold,out})}{2} \right) \right)^{1/3}$	(3.114)

ii) Organic Rankine Cycle (ORC) Components

The Cycles package included in the ThermWatt library (at the time of the development of this work) contains a sub-package for the equipment existing in the Organic Rankine Cycle (ORC) system. In Tables 3-22 and 3-23, the equipment-level models included in an ORC are characterized.

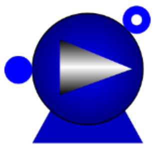
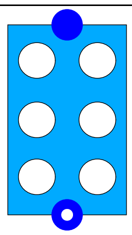
Table 3-22. Characterization of ORC equipment models (Heat exchanger units)

Heat recovery steam generator (HRSG) Unit	
Category within the library	New
	It is a component that represents the heat recovery steam generator technology constituted by an economiser (heats up the liquid stream to the boiling point), an evaporator (it processes the phase change of the liquid stream to the point that all of the initial quantity of liquid is on the vapour phase) and a superheater (heats up the stream to a temperature considerably above the boiling temperature); While the thermodynamic cycle working fluid constitutes the cold stream, a gas stream constitutes the hot stream; It is modelled to ensure that all the inlet liquid stream is converted to the vapour phase (by allocating the necessary enthalpy withdrawn from the hot stream); It considers as necessary parameters: • Superheater overall heat transfer coefficient;

	• Superheated heat transfer area. The model is generally described by the equations presented below, resulting as an adaption of the equations presented in Table 3-10.	
Hot Gas-side	$\dot{M}_{Gas,in} = \dot{M}_{Gas,out}$	(3.115)
	$\dot{M}_{Gas,in} \cdot h_{Gas,in} = \dot{M}_{Gas,out} \cdot h_{Gas,out} + q_{HT}$	(3.116)
Organic Fluid-side	$\dot{M}_{Org,in} = \dot{M}_{Org,out}$	(3.117)
	$\dot{M}_{Org,in} \cdot h_{Org,in} + q_{Econ.} = \dot{M}_{Org,out} \cdot h_{Org,L}$	(3.118)
	$\dot{M}_{Org,in} \cdot h_{Org,L} + q_{Evap.} = \dot{M}_{Org,out} \cdot h_{Org,V}$	(3.119)
	$\dot{M}_{Org,in} \cdot h_{Org,V} + q_{SuperH.} = \dot{M}_{Org,out} \cdot h_{Org,out}$	(3.120)
Hear Transfer	$q_{HT} = q_{Econ.} + q_{Evap.} + q_{SuperH.}$	(3.121)
	$\dot{M}_{Org,in} \cdot h_{Org,in} + q_{Econ.} = \dot{M}_{Org,out} \cdot h_{Org,L}$	(3.122)
	$q_{SuperH.} = U \cdot A \cdot \Delta T_{med}$	(3.123)
	$\Delta T_{med} = \left((T_{Hot,in} - T_{Cold,out}) \cdot (T_{Hot,out} - T_{Cold,in}) \cdot \left(\frac{(T_{Hot,in} - T_{Cold,out}) + (T_{Hot,out} - T_{Cold,in})}{2} \right) \right)^{1/3}$	(3.124)
Regenerator		
Category within the library	New	
	It is a component that represent an ORC regenerator operating in counter-current operation; It considers as necessary parameters: • Overall heat transfer coefficient; • Heat transfer area; • Pressure loss relative to the liquid-side; The model is generally described by the equations presented below, resulting as an adaption of the equations presented in Table 3-10.	
Vapour-side	$\dot{M}_{Hot,in} = \dot{M}_{Gas,out}$	(3.125)
	$\dot{M}_{Gas,in} \cdot h_{Gas,in} = \dot{M}_{Gas,out} \cdot h_{Gas,out} + q_{HT}$	(3.126)
Liquid-side	$\dot{M}_{Cold,in} = \dot{M}_{Cold,out}$	(3.127)
	$\dot{M}_{Cold,in} \cdot C_{Cold,in} = \dot{M}_{Cold,out} \cdot C_{Cold,in}$	(3.128)
	$\dot{M}_{Cold,in} \cdot h_{Cold,in} + eff_{HT} \cdot q_{HT} = \dot{M}_{Cold,out} \cdot h_{Cold,out}$	(3.129)
	$p_{in} = p_{out} + \Delta p$	(3.130)
Heat Transfer	$q_{HT} = U \cdot A \cdot \Delta T_{med}$	(3.131)
	$\Delta T_{med} = \left((T_{Hot,in} - T_{Cold,in}) \cdot (T_{Hot,out} - T_{Cold,out}) \cdot \left(\frac{(T_{Hot,in} - T_{Cold,in}) + (T_{Hot,out} - T_{Cold,out})}{2} \right) \right)^{1/3}$	(3.132)
Condenser		
Category within the library	New	
	It is a component that represents a condenser installed in an ORC; While the ORC working fluid constitutes the hot stream, a separated liquid stream constitutes the cold stream; Two version of this model exist: one considering both the hot and cold streams and another considering only the hot stream (used in cases in which the auxiliary cooling circuit of the ORC is not set to be assessed in detail); It is modelled so to ensure that all the quantity of the inlet gas stream is converted to the liquid phase through phase change, as expressed in the equations below.	
Organic Fluid-side	$\dot{M}_{Org,in} = \dot{M}_{Org,out}$	(3.133)
	$\dot{M}_{Org,in} \cdot h_{Org,V} = \dot{M}_{Org,L} \cdot h_{Org,L} + q_{HT}$	(3.134)
Cooling	$\dot{M}_{Cool.,in} = \dot{M}_{Cool,out}$	(3.135)

fluid-side	$$\dot{M}_{Cool.,in} \cdot h_{Cool,in} + q_{HT} = \dot{M}_{Cool.,out} \cdot h_{Cool,out} \quad (3.136)$$

Table 3-23. Characterization of ORC equipment models (Additional equipment)

Centrifugal pump	
Category within the library	New
	It is a component that represents a centrifugal pump installed in liquid transportation circuits (in the case of the ORC, the organic working fluid); It considers as necessary parameters: • The outlet pressure or the mass flow rate (one of the these must alternately be defined); • Hydraulic efficiency; • Mechanical efficiency; The mass and enthalpy relative to this model are expressed by equations (3.137) and (3.138), while the pressure balance calculated considering the aforementioned parameters is expressed by equation (3.139).
$$\dot{M}_{Org,in} = \dot{M}_{Org,out}$$	(3.137)
$$\dot{M}_{Org,in} \cdot h_{Org,in} = \dot{M}_{Org,out} \cdot h_{Org,out}$$	(3.138)
$$Pot_{pump} \cdot \eta_{hydr.} \cdot \eta_{mech} = \frac{\dot{M}_{Org}}{\rho_{Org}} \cdot (p_{Org,out} - p_{Org,in})$$	(3.139)
Cooling Tower	
Category within the library	New
	It is a component that represents a cooling tower installed in the auxiliary cooling circuit of an ORC; It is modelled so to ensure that the inlet liquid stream is cooled down to a defined outlet temperature, so to ensure the overall enthalpy balance of the auxiliary circuit (in which the inlet total enthalpy corresponds to outlet total enthalpy), as defined by the mass and enthalpy equations below.
$$\dot{M}_{Cool.,in} = \dot{M}_{Cool,out}$$	(3.140)
$$\dot{M}_{Cool.,in} \cdot h_{Cool,in} = \dot{M}_{Cool.,out} \cdot h_{Cool,out} + q_{HT}$$	(3.141)

iii) Thermal Energy Storage

The *Storage* package of the ThermWatt Modelica library contains the required component models for the modelling of TES systems, mainly including the TES units themselves. While the system-level components are generally developed from adaptations of the components present in the *General* package, the TES units models are exhaustively developed, taking into account the accurate occurrence of the heat transfer phenomena. In Table 3-24, the model developed for the phase change material (PCM)-based heat exchanger is characterized.

Table 3-24. Characterization of thermal energy storage models

PCM-based Heat Exchanger	
Category within the library	New

It is a component that represents a PCM-based heat exchanger, in which a waste heat gas stream is the heat source and an air stream is the heat sink;

It considers the input of three types of parameters: PCM properties-related parameters and heat exchanger geometry-related parameters and setup parameters (initial conditions for simulation);

In relation to PCM properties-related parameters, it considers the input of:

- PCM thermal conductivity (solid and liquid phase);
- PCM specific heat capacity (solid and liquid phase);
- PCM density (solid and liquid phase);

In relation to heat exchanger geometry-related parameters, it considers the input of:

- Length of the shell and tubes side;
- Internal diameter of exhaust gas/ air contact tubes;
- External diameter of exhaust gas/ air contact tubes;
- Number of total exhaust gas/ air contact tubes;

In relation to setup parameters, it considers the starting temperature of the PCM-side (which is the setup PCM temperature at time zero);

The model is generally described by the equations presented below, resulting as an adaption of the equations presented in Table 3-11;

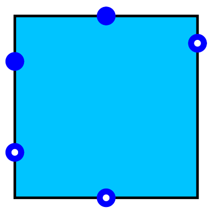
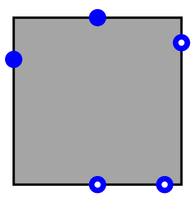
The obtainment of the equations describing conductive heat transfer is characterized in appendix A2, while the obtainment of the equations for the determination of PCM properties in phase change is characterized in appendix A3 (in which it is considered a method of computation of the PCM properties according to empirical methods using the Gauss error function [375], which in the case of this model is approximated using an analytical function [376]).

PCM Side	**General**	$\alpha_{i,j} \cdot \left(\frac{1}{r_{i,j}} \cdot \left(\frac{T_{i,j+1} - T_{i,j-1}}{r_{i,j+1} - r_{i,j-1}} \right) + \left(\frac{T_{i,j+1} - 2 \cdot T_{i,j} + T_{i,j-1}}{\left(r_{i,j+1} - r_{i,j+1}\right)^2} \right) \right) = \frac{dT}{dt}_{i,j}$	(3.142)
		$\alpha_{i,j} = \frac{k_{i,j}}{\rho_{i,j} \cdot C_{P_{i,j}}}$	(3.143)
	Solid Phase	$C_{P,app,i,j} = C_{P,s}$	(3.144)
		$k_{i,j} = k_s$	(3.145)
		$\rho_{i,j} = \rho_s$	(3.146)
	Phase Change	$C_{P,app,i,j} = \frac{\Delta h_{Cond.}}{(2 \cdot \pi)^{0.5} \cdot \tau} \cdot \exp\left(\frac{-\left(T_{i,j} - T_S\right)^2}{2 \cdot \tau^2} \right) + C_{P,S} + \left(C_{P,L} - C_{P,S}\right) \cdot 0.5 \cdot \left(1 + \left(-1 + \frac{2}{1 + \exp\left(-2.5 \cdot \left(\frac{\left(T_{i,j} - T_S\right)}{\sqrt{2} \cdot \tau} \right) \right)} \right) \right)$	(3.147)
		$k_{i,j} = k_s + (k_l - k_s) \cdot 0.5 \cdot \left(1 + \left(-1 + \frac{2}{1 + \exp\left(-2.5 \cdot \left(\frac{\left(T_{i,j} - T_S\right)}{\sqrt{2} \cdot \tau} \right) \right)} \right) \right)$	(3.148)
		$\rho_{i,j} = \rho_s + (\rho_l - \rho_s) \cdot 0.5 \cdot \left(1 + \left(-1 + \frac{2}{1 + \exp\left(-2.5 \cdot \left(\frac{\left(T_{i,j} - T_S\right)}{\sqrt{2} \cdot \tau} \right) \right)} \right) \right)$	(3.149)
	Liquid Phase	$C_{P,app,i,j} = C_{P,l}$	(3.150)
		$k_{i,j} = k_l$	(3.151)
		$\rho_{i,j} = \rho_l$	(3.152)
Heat Source/ Sink Side		$\dot{M}_{Gas_i} = \dot{M}_{Gas_{i+1}}$	(3.153)
		$q_{Gas_i} = \dot{M}_{Gas_i} \cdot \left(T_{Gas_i} - T_{Gas_{i+1}}\right)$	(3.154)
		$q_{Gas_i} = \sum_{j=1}^{M} \frac{dH_{Stored}}{dt}_{i,j}$	(3.155)

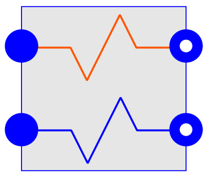
3.3.3. Models for Heat-driven Wastewater Treatment Technologies

The *Wastewater Treatment* package of the ThermWatt Modelica library contains a sub-package dedicated to the equipment-level models constituent of a Multi-effect distillation (MED Unit). In Table 3-25, the equipment-level models of this category area characterized.

Table 3-25. Characterization of heat-driven wastewater treatment component models

MED Effect 1		
Category within the library	New	
	It is a component that represents an effect of a MED unit, namely the first effect in which an external heat source stream (in this case, a gas stream) constitutes the hot stream and the wastewater stream constitutes the cold stream; It is modelled so to the inlet quantity of water stream is heated up to the boiling point temperature and it is furtherly heated up so a determinate quantity of it is converted to the vapour phase (determined by the quantity of withdrawn enthalpy from the heat source stream); It considers as necessary parameters: • Overall heat transfer coefficient; • Heat transfer area; The model is generally described by the equations presented below, resulting as an adaption of the equations presented in Table 3-12.	
Water-side	$\dot{M}_{W,1} = \dot{M}_{V,1} + \dot{M}_{B,1}$	(3.156)
	$\dot{M}_{W,1} \bullet C_{W,1} = \dot{M}_{B,1} \bullet C_{B,1}$	(3.157)
	$\dot{M}_{W,1} \bullet h_{W,1} + q_{MED} = \dot{M}_{V,1} \bullet h_{V,1} + \dot{M}_{B,1} \bullet h_{w,L}$	(3.158)
Hot Gas-side	$\dot{M}_{Gas,in} = \dot{M}_{Gas,out}$	(3.159)
	$\dot{M}_{Gas,in} \cdot h_{Gas,in} = \dot{M}_{Gas,out} \cdot h_{Gas,out} + q_{MED}$	(3.160)
Heat Transfer	$q_{HT} = U \cdot A \cdot \Delta T_{med}$	(3.161)
	$\Delta T_{med} = \left((T_{Hot,in} - T_{Cold,in}) \cdot (T_{Hot,out} - T_{Cold,out}) \cdot \left(\frac{(T_{Hot,in} - T_{Cold,in}) + (T_{Hot,out} - T_{Cold,out})}{2} \right) \right)^{1/3}$	(3.162)
MED Effect k		
Category within the library	New	
	It is a component that represents an effect of a MED unit, namely the second-to-last effects in which the vapour stream at the outlet of the immediately previous effect constitutes the hot stream and the wastewater stream constitutes the cold stream; It is modelled so to the inlet quantity of water stream is heated up to the boiling point temperature and it is furtherly heated up so a determinate quantity of it is converted to the vapour phase (determined by the quantity of withdrawn enthalpy from the heat source stream); It considers as necessary parameters: • Overall heat transfer coefficient; • Heat transfer area; The model is generally described by the equations presented below, resulting as an adaption of the equations presented in Table 3-12.	
Water-side	$\dot{M}_{W,k} = \dot{M}_{V,k} + \dot{M}_{B,k}$	(3.163)
	$\dot{M}_{W,k} \bullet C_{W,k} = \dot{M}_{B,k} \bullet C_{B,k}$	(3.164)
	$\dot{M}_{W,1} \bullet h_{W,1} + q_{MED,k} = \dot{M}_{V,1} \bullet h_{V,1} + \dot{M}_{B,1} \bullet h_{w,L}$	(3.165)

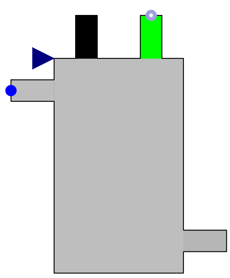
Vapour-side	$\dot{M}_{V,k-1} = \dot{M}_{TW,k-1}$	(3.166)
	$\dot{M}_{V,k-1} \cdot h_{V,k-1} = \dot{M}_{TW,k-1} \cdot h_{W,L} + q_{MED,k}$	(3.167)

MED Condenser		
Category within the library	New	
	It is a component that represents the condenser of a MED unit, in which the vapour stream from the last effect is the hot stream and the inlet wastewater stream is the cold stream; It is modelled to ensure that all the inlet quantity of vapour is converted to the liquid phase (namely to the limit specific enthalpy of the liquid phase); The model is generally described by the equations presented below, resulting as an adaption of the equations presented in Table 3-12.	
Water-side	$\dot{M}_{WW,in} = \dot{M}_{WW,out}$	(3.168)
	$\dot{M}_{WW,in} \bullet C_{WW,in} = \dot{M}_{WW,out} \bullet C_{WW,out}$	(3.169)
	$\dot{M}_{WW,in} \bullet h_{WW,in} + (q_{MED,Cond} - q_{MED,Losses}) = \dot{M}_{WW,out} \bullet h_{WW,out}$	(3.170)
Vapour-side	$\dot{M}_{V,N} = \dot{M}_{TW,N}$	(3.171)
	$\dot{M}_{V,N} \cdot h_{V,N} = \dot{M}_{TW,N} \cdot h_{W,L} + q_{MED,Cond}$	(3.172)

3.3.4. Models for Wastewater-to-energy Technologies

The wastewater-to-energy technologies approached in this work are modelled within the framework of the ThermWatt library as part of the *WWtE* package. This package contains models considering the inlet of a discharge water stream (with variable concentration of contaminants, such as discharged treated water from a water system or the sludge stream from a wastewater treatment unit) and an outlet of a generated fuel stream (such as hydrogen). As mentioned, at the time of the development of this work only the model of an Electrolysis unit has been developed. In Table 3-26, the equipment-level model of this category is characterized.

Table 3-26. Characterization of wastewater-to-energy models

Electrolysis Unit		
Category within the library	New	
	It is a component that represents a generic electrolysis unit, in which a determinate quantity of water is converted to hydrogen and oxygen; It considers an inlet port for the inlet water stream and the outlet produced hydrogen stream, with the streams for the non-converted quantity of the inlet water stream and outlet produced hydrogen being only considered through calculations; It also considers an inlet port for electricity; It considers the input of the single parameter of electricity conversion into effectively used reaction enthalpy ($eff_{conversion}$); The quantity of produced hydrogen is variable, depending on the quantity of inlet electric energy, as expressed in the equations below.	
	$\dot{M}_{In} \cdot eff_{Electr.} = \dot{M}_{H_2}$	(3.173)
	$q_{required} \cdot eff_{Electr.} = Pot_{supply} \cdot eff_{conversion}$	(3.174)
	$q_{required} = \dot{M}_{W,In} / PM_W \cdot \Delta H^0{}_{WSp.}$	(3.175)

3.4. Validation of Equipment-level Models

The equipment-level models presented in section 3.3 have been developed according to governing equations generally gathered from existing literature, with a small set of models subsisting on empirical observations with the imperative of the simplification of the modelling of the occurring physical phenomena. These models have to be validated so to be furtherly part of the system-level models to be simulated to each one of the case-studies approached in this work. As mentioned before, a part of the approached component models has been developed according to significant simplifications regarding the occurrence of physical phenomena, which is considered a valid procedure as the models to be of effective importance are the system-level models. As such, the referred models do not need an exhaustive validation procedure, as the simulation of the occurring phenomena is simplified to that point. Nonetheless, the Modelica library does contain a set of models whose simulated phenomena are modelled to such a sufficient detail for the performance of such validation procedure not to be relevant.

In the scope of these work, the following equipment-level models have been validated:

- Tunnel Kiln (validated with plant data);
- Organic Rankine Cycle (ORC) (validated with plant data);
- PCM-based heat exchanger (validated with literature data);
- Multi-effect distillation (MED) (validated with literature data).

The validation procedure is performed by assessing the relative deviation associated to each key variable characterizing the model. The general formula considered for the calculation the relative deviation is expressed by equation (3.176), which considers a number of N measurements for a same variable (such as the ones corresponding the different values associated to a variable for each instant of time).

$$\mathrm{ARD} = \frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}} \frac{\left|\mathrm{M}_{\mathrm{exp,i}} - \mathrm{M}_{\mathrm{sim,i}}\right|}{\mathrm{M}_{\mathrm{exp,i}}} \tag{3.176}$$

Tunnel Kiln model

The tunnel kiln model works with the necessary input of certain parameters associated to the fuel, combustion air, produced material and cooling air/ hot air streams. In total, these parameters are:

- Mass flow rate of fuel;
- Inlet temperature of fuel;
- Inlet temperature of ambient air;
- Ait-to-fuel ratio;
- Mass flow rate of produced material;
- Inlet temperature of produced material;
- Outlet temperature of produced material;

- Mass flow rate of cooling air/ hot air;
- Inlet temperature of cooling air;
- Outlet temperature of hot air.

Following the mathematical formulation of the mass and enthalpy balance equation for the tunnel kiln, the following variables are set as key variables to characterize the validation procedure for this model:

- Mass flow rate of the combustion air stream.
- Mass flow rate of the exhaust gas stream;
- Temperature of the exhaust gas stream.

In this sense, a test model was developed for the purpose of the validation of the developed model, whose flowsheet representation is presented in Figure 3.9. In respect to the test model pictorially represented, the following initial procedure was performed for the propose of validation:

- The combustion air stream corresponds to the ambient air, with this stream being allocated to one of the air entrance ports in the tunnel kiln model;
- To the secondary air entrance port (which is generally set to be used for the inlet of the recirculated hot air) was connected an air source whose mass flow rate was set as null;
- To each one of the aforementioned input parameters, the values associated to an existing ceramic plant are considered.

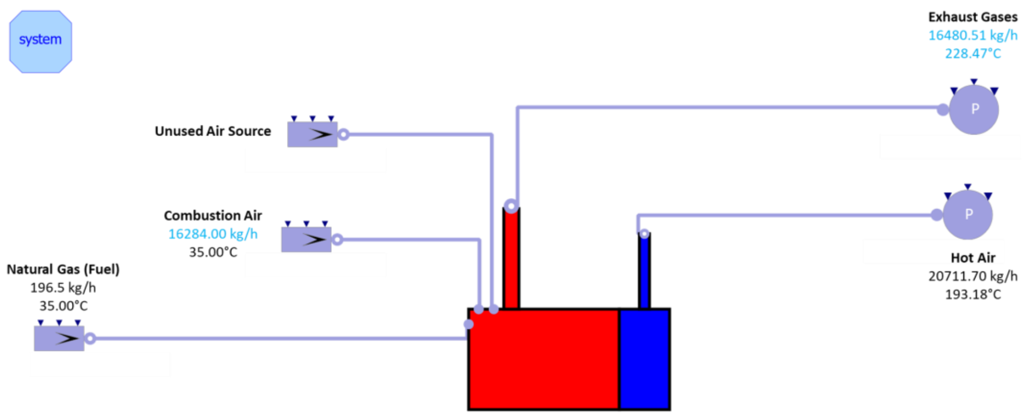


Figure 3.9. Test model for the validation of the Tunnel kiln component model (to-be-validated key variables are signalized in a lighter colour)

From the mentioned procedure and the simulation of the model represented in Figure 3.9, it resulted a set of simulated values that may be compared to real plant measured ones. In Table 3-27, the comparison of real and simulated values in terms of the determination of relative deviation to the tunnel kiln model is presented.

Table 3-27. Determination of the deviation associated to key variables for the Tunnel kiln model

Variable	Real Value	Simulated Value	ARD
Mass flow rate of	16284.00	16284.00	0.00%

combustion air (kg/h)			
Mass flow rate of exhaust gases (kg/h)	16480.70	16480.51	0.00%
Temperature of exhaust gases (ºC)	230.00	228.47	0.67%

As may be verified by the analysis of Table 3-27, the obtained deviations present only residual values for all the analysed key parameters. The mass flow rate of combustion air, only depending on the input of two parameters (mass flow rate of fuel and air-to-fuel ratio), presents an exact correspondence. The mass flow rate of the exhaust gases presents a negligible difference, which may be associated to the uncertainty associated to the flowmeter that was used for measuring such quantity considered as the real value. The temperature of exhaust gases presents a small difference which may be associated to the different gas compositions considered for the respective media packages in comparison to the actual gas compositions (namely the default gas compositions for natural gas, air and exhaust gases).
Taking into account the presented results, the tunnel kiln model may be considered valid and as such apt to be used in system-level models.

Organic Rankine Cycle (ORC) model

The Organic Rankine Cycle (ORC) model is roughly a system-level model considering the assembly of several component models. For the effects of the performance of the validation procedure, the ORC model will be assessed as an integrate (the system-level model as a whole and not each one of the components). Such procedure is taken since this model is also set to be included in the integrate within the system-level models of each one of the case-studies. The following parameters are set as inputs:

- Mass flow rate of heat source stream (exhaust gases);
- Inlet temperature of heat source stream (exhaust gases);
- Outlet temperature of heat source stream (exhaust gases);
- Mass flow rate associated to the auxiliary cooling water cycle;
- Power consumption associated to the cooling water cycle pump;
- Heat duty in the cooling tower.

The following variables were set as key variables to be analysed in the validation procedure:

- Temperature of the water stream at the inlet of the condenser;
- Temperature of the water stream at the outlet of the condenser;
- Power consumption associated to the main cycle pump;
- Generated electricity (in the generator connected to the turbine).

A test model was developed for the purpose of the validation of the developed ORC model (in which the working organic fluid is NOVEC649), whose flowsheet representation is presented in Figure 3.10.

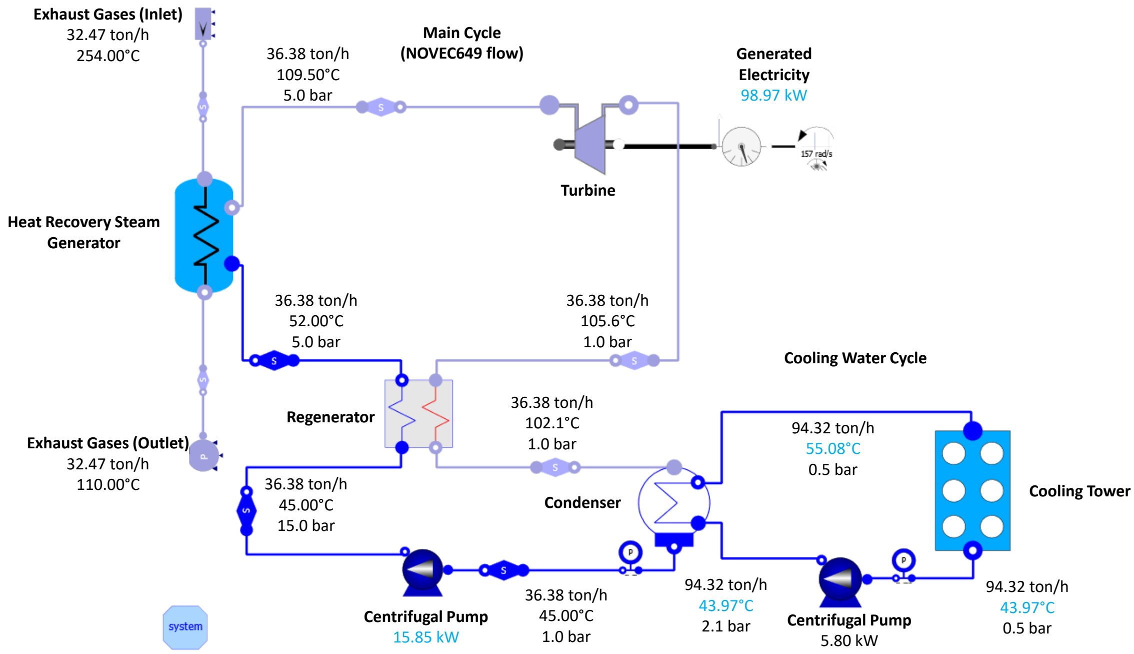


Figure 3.10. Test model for the validation of the Organic Rankine Cycle (ORC) system model (to-be-validated key variables are signalized in a lighter colour)

In Table 3-28, the comparison of real and simulated values in terms of the determination of relative deviation to the ORC model is presented.

Table 3-28. Determination of the deviation associated to key variables characterizing the ORC model

Variable	Real Value	Simulated Value	ARD
Temperature of the Water Stream at the Inlet of the Condenser (ºC)	44.00	43.97	0.07%
Temperature of the Water Stream at the Outlet of the Condenser (ºC)	54.00	55.08	2.00%
Power Consumption associated to the main cycle pump (kW)	16.00	15.85	0.94%
Generated Electricity (kW)	99.80	98.97	0.83%

As may be verified by the analysis of Table 3-28, the obtained deviation values are considerably low. All the key parameters (in the exception of the Temperature of the Water Stream at the Outlet of the Condenser) present deviation lower than 1%, which are highly acceptable. As for the parameter identified as an exception, such considerably higher deviation may be attributed to the determination of the heat duty to be inputted to the cooling tower. Such heat duty value corresponds to the total enthalpy allocated from the organic fluid stream circulating in the main cycle to the water stream within the cooling water cycle, for the purpose of maintaining the enthalpy balance within the water cycle assuming the inexistence of heat losses. In its turn, this heat duty is influenced by the condensation enthalpy associated to the organic fluid (which in turn depends on the specific enthalpies of saturated liquid and saturated steam, considered as constants within the definition of the medium package) and the enthalpy associated to the temperature decrease from the inlet temperature to the boiling point temperature (52.00ºC). While the vaporization enthalpy is considered as a constant by model definition, the second term depends on the outlet temperature from the regenerator. In this sense, the verified difference in relation to the heat duty (and, as such, the water temperature) may be attributed either to a difference in terms of the considered vaporization enthalpy or the definition of the values attributed to the parameters associated to the regenerator that permit the output of a temperature of the corresponding hot stream (the organic fluid in the gas phase) of 70.40ºC. Taking into account these considerations, and at the light of the obtained simulated value, such deviation may be considered overall acceptable.

Taking into account the presented results, the ORC model may be considered valid and as such apt to be used in system-level models.

PCM-based heat exchanger model

The PCM-based heat exchanger equipment model is planned to be inserted in system-level models set for dynamic simulation (this is, accounting for the existence of significant variations associated to some variables along with time). As such, the comparison between corresponding theoretical and simulation values for this component must be performed by the comparison of the time-variating plots associated to the key variables. The deviation associated to such comparison is then calculated by the most general formula expressed by equation (3.176), in which the number of total measurements correspond to the number of simulation points (which in its turn is determined by the total simulation time and the time step).

For the performance of the simulation procedure, the following parameters are set as inputs:

- Mass flow rate of heat source stream (exhaust gases);
- Inlet temperature of heat source stream (exhaust gases);
- Geometric-related parameters of the PCM-based heat exchanger (internal radius, external radius and length);
- Initial temperature of the PCM.

The following variables were set as key variables to be analysed in the validation procedure:

- Temperature of PCM (along with time) for the enthalpy charge (supply of the heat source stream);
- Temperature of PCM (along with time) for the enthalpy discharge (supply of heat sink stream).

A test model was developed for the purpose of the validation of the developed PCM-based heat exchanger model. For the purpose of the validation of two different phenomena associated to thermal energy storage (enthalpy chare and discharge), two different simulations were proceeded using the same test model:

- One for the charge phase (attribution of values for the heat source stream);
- Other for the discharge phase (attribution of values for the heat sink stream).

The flowsheet representation for the test model is presented in Figure 3.11. The simulation setup in terms of the definition of the simulation time is presented in Table 3-29. The setup values (gathered from the reference literature [377] used for the validation of this model) for the key variables that define the PCM-based heat exchanger component and the heat source and heat sink streams are presented in Table 3-31, respectively. The obtained relative deviations associated to two simulations are presented in Table 3-32. The literature and simulation time-variating plots for the PCM temperature during the charge phase are presented in Figure 3.12.

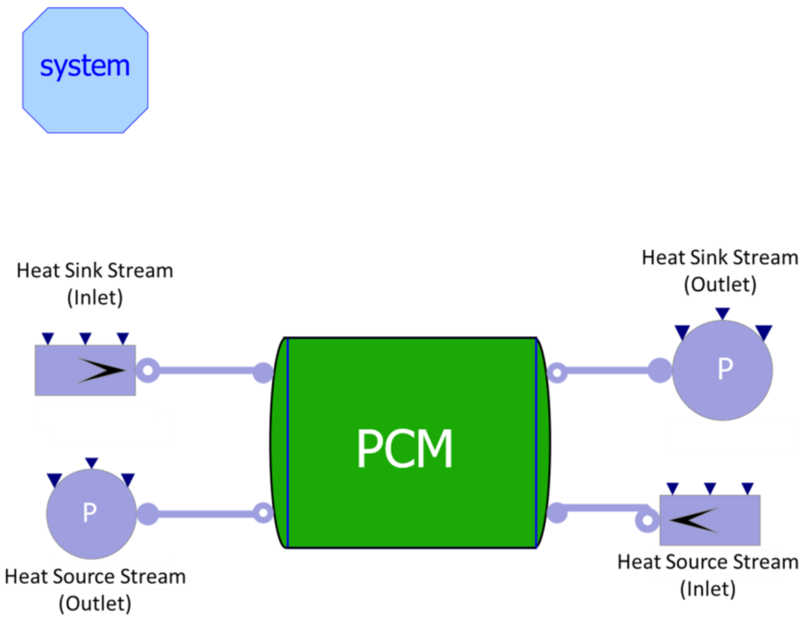


Figure 3.11. Test model for the validation of the PCM-based heat exchanger

Table 3-29. Simulation setup for the PCM-based heat exchanger test model

Parameter	Value	
	Enthalpy Charge Simulation	**Enthalpy Discharge Simulation**
Start Time (s)	0	0
Stop Time (s)	31200	54000
Number of Time Intervals	31200	54000

Table 3-30. Setup values related to PCM-based heat exchanger component

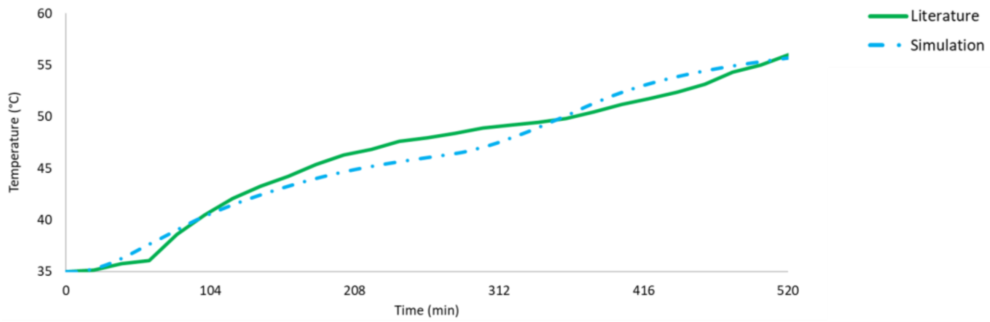
Geometric parameters for the PCM-based heat exchanger	
Length (m)	1.000
Internal Radius (m)	0.0125
External Radius (m)	0.0635
PCM physical properties	
Melting/ Solidification lower limit temperature (ºC)	41
Melting/ Solidification upper limit temperature (ºC)	55
Melting/ Solidification latent enthalpy (J/kg)	176000
Solid/ Liquid phase specific heat capacity (J/(ºC.kg))	2800
Solid/ Liquid phase density (kg/m^3)	835
Solid/ Liquid phase conductive heat transfer coefficient (W/(ºC.m))	0.21

Table 3-31. Setup values for stream parameters

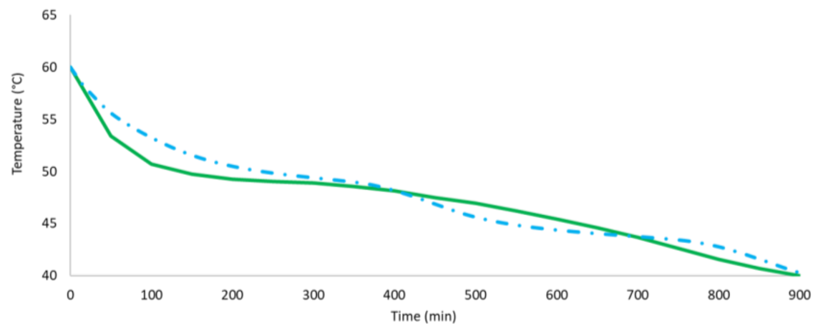
Phase	Stream	Mass Flow Rate (kg/h)	Inlet Temperature (ºC)	Initial PCM Temperature (ºC)
Charge	Heat Source Stream	10.80	90.00	35.00
Discharge	Heat Sink Stream	10.80	30.00	60.00

Table 3-32. Relative deviation obtained for the Charge and Discharge phase models

Phase	ARD
Charge	2.16%
Discharge	2.12%



a)



b)

Figure 3.12. Comparison of profiles for the inside PCM temperature between literature and simulation for a) the enthalpy charge phase, b) enthalpy discharge phase

As may be verified by the analysis of Figure 3.12 – a), the profiles corresponding to literature and simulation results effectively for the enthalpy charge phase generally present the same tendency in terms of temperature variation. Nonetheless, it is possible to observe slight differences in terms temperature variation in determinate sets of simulation time intervals, which may be effectively verified by two intersections points between both temperature profiles. Such deviation is more pronounced on the simulation points in which the temperature is more proximate to the phase change interval (41 – 55ºC). In this prospect, such occurrence may be attributed to the use of different methods for the computation of the PCM temperature between the corresponding literature model and the model developed for this work.

In relation to the temperature profiles obtained for the enthalpy discharge phase, it is possible to appoint similar verifications for this simulation based on the analysis of Figure 3.12 – b). Two intersections points between the literature and simulations temperature profiles are visible and the most significant deviations are obtained for simulation points in which the temperature is more proximate to the phase change interval.

Taking into account the obtained mean deviation values between the temperature profiles of literature and the performed simulations (which in terms of accuracy assessment may be considered acceptable values), it may be affirmed that the literature and simulation temperature profiles for both simulations are consistent and the model is valid, and thus set to be integrated in system-level simulation.

Multi-effect distillation (MED) unit model

The Multi-effect distillation (MED) model required to be developed consists in the assembling of the equipment-level models of the First effect, Second-to-last effect and Condenser presented in section 3.3.3. The MED system-level model is set to be validated against literature data gathered from the Rahimi and Chua [360], in which the MED technology is profoundly characterized and in which a modelling framework is established. The overall model developed by Rahimi and Chua is characterized by several assumptions, which are also considered for each of the equipment-level models of First effect, Second-to-last effect and Condenser and the whole MED model developed in the scope of this work. In Table 3-33, the assumptions taken by Rahimi and Chua are described, being divided in three categories: heat losses-related, stream parameters-related and constant value definition-related.

Table 3-33. Modelling assumptions taken by Rahimi and Chua [360]

Category	Assumption
Heat Losses	• The heat losses in each effect and the flashing chamber are negligible; • The heat losses associated to the vapor flow (in the demister, transmission lines and condensation inside tubes) are negligible.
Stream parameters	• The operational pressure of the condensation process is constant; • The pressure losses of the vapor flow (in the demister, transmission lines and condensation inside tubes) are negligible; • The temperature and salinity of the inlet wastewater stream (feed water) are constant • The outlet treated water stream is considered pure (null salinity).
Specific values	• The pressure difference for injecting vapor from the flashing chambers is set at 0.005 bar (for all relevant MED effects); • In the primary MED effects, a temperature difference of 2.5 ºC between the condensed vapour and the outlet concentrate streams is considered.

For the purpose of the validation of the MED model, literature data gathered from Rahimi and Chua [360] is used, namely one for an installation for seawater desalination in which the heat source stream is water and integrating a total of four effects. The consideration of a different heat source stream within the First effect model presented in section 3.3.3 serves for the purpose of the validation, since the set of equations is not changed.

For the running of the test model, the following parameters are set as inputs:

- Mass flow rate of inlet saline water;
- Concentration of contaminant (salt) of the inlet saline water
- Mass flow rate of purged saline water at the outlet of the condenser;
- Temperature of the saline water stream at the outlet of the condenser;
- Mass flow rate of the heat source stream;
- Inlet temperature of the heat source stream;
- Outlet temperature of the heat source stream;
- Pressure of the treated water streams at the outlet of each effect/ condenser.

The following variables were set as key variables to be analysed in the validation procedure:

- Mass flow rate of the treated water stream (resulting from the mixing of all the distillate streams at the outlet of each effect/ condenser);
- Temperature of the vapour stream at the outlet of each effect.

A test model was developed for the purpose of the validation of the developed MED model, whose flowsheet representation is presented in Figure 3.13.

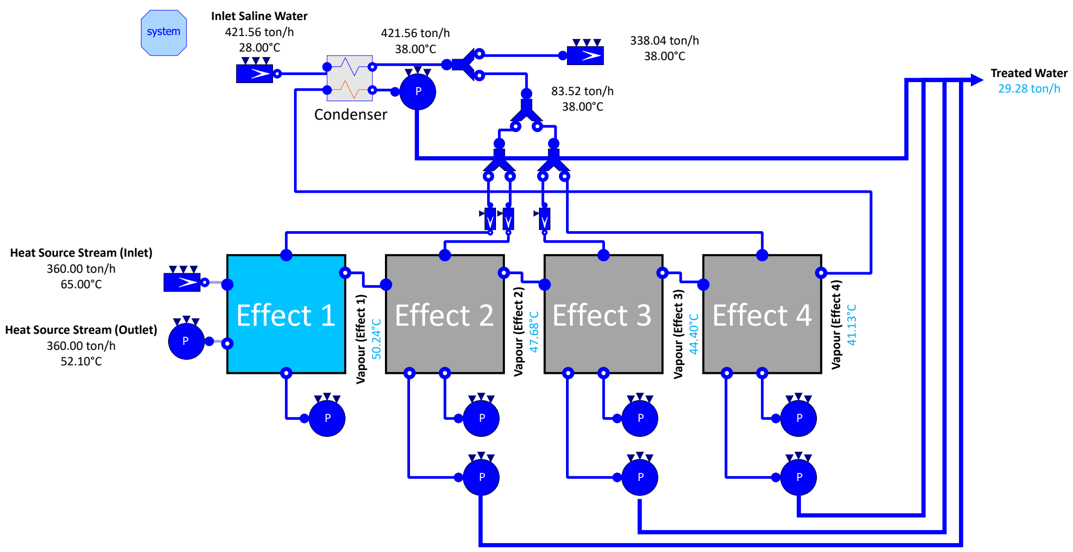


Figure 3.13. Test model for the validation of the Multi-effect distillation (MED) system model (to-be-validated key parameters are signalized in a lighter colour)

In Table 3-34, the comparison of real and simulated values in terms of the determination of relative deviation to the ORC model is presented.

Table 3-34. Determination of the deviation associated to key variables characterizing the Multi-effect distillation (MED) model

Variable	Literature Value	Simulated Value	ARD
Mass flow rate of treated water stream (kg/h)	28800	29275.74	1.65%

Temperature of the vapour stream at the outlet of Effect 1	50.30	50.24	0.12%
Temperature of the vapour stream at the outlet of Effect 2	47.20	47.68	1.02%
Temperature of the vapour stream at the outlet of Effect 3	44.10	44.40	0.68%
Temperature of the vapour stream at the outlet of Effect 4	41.10	41.13	0.07%

As may be verified by the analysis of Table 3-34, the deviations obtained for the MED test model present significantly low deviations in comparison to the respective literature values. It is to note that the values obtained for the temperature of the vapour stream at the outlet of each effect depend on the pressure of the vapour stream at the outlet of each effect, which in this case is determined by the pressure of the treated water streams at the outlet of the immediately next effect/ condenser (taking into account that pressure losses are considered negligible). In its turn, the relation between the vapour stream temperature (boiling point temperature) and the pressure do also vary on the used computational package for water properties (while the Modelica package for Water uses the IF97 steam/ water properties package, Rahimi and Chua [360] use REFPROP). While the values obtained for these temperature parameters are overall consistent with the respective literature data, the definition of pressure values that are more proximate to the ones corresponding to the exactly correct vapour boiling point temperature values according to the steam/ water properties package used by ThermWatt (which is the IF97 standardly used by Modelica) would allow the obtainment of even more accurate values. Even more accurate values for these temperatures would also make possible the obtainment of a more accurate value for the mass flow rate of the treated water stream. Nevertheless, regarding the overall significantly low deviations obtained for the key variables, such details may be considered unnecessary for the validation procedure, and the MED model may be considered valid, and as such apt to be used in system-level models.

3.5. Definition of Post-processing Indicators

The post-processing procedure performed through the assessment of results from the models developed with the capabilities of the ThermWatt computational tool consist in general on the estimation of indicators related to sustainability promotion. In a primary phase, these indicators are set to assess the economic viability and environmental impact reduction potential associated to the conceptualized Water and Energy Integration Systems (WEIS) as Engineering projects. These are indicators that directly assess the viability of the WEIS projects, being determined by the direct analysis of the optimisation results (in addition to the estimation of investment costs for the installation). In a further phase, two other sets of indicators are set to be estimated: one related to the eco-efficiency promotion and another related to circular economy character promotion (related to the passage from open-loop to closed-loop systems). These last not only serve to reinforce the viability of the proposed WEIS but also to prove the self-sufficiency of these in terms of exploitation of energy and water resources and the production of economic value. In general, these indicators are adaptations of the sustainability assessment indicators characterized in section 2.6 to the paradigms of the WEIS and the case-studies that will be furtherly presented. Another set of indicators are enunciated by considering ratios between values that are obtained by direct observation of the energy system installed in the plant, freshwater consumption and the quantities of discharge water.

In Table 3-35, the first sets of indicators are defined, with the respective calculation formulas being demonstrated. In the sequence of Tables 3.36 and 3.37, the second sets of indicators are characterized (these indicators are defined with the exact units that are set to be used in the post-processing assessment). In Table 3-38, the formulas used to determine the most basic indicators of economic savings and equivalent carbon dioxide emissions are defined. In both the calculation formulas, the index i represents a certain energy source in which the WEIS is conceptualized to reduce the emission level (for instance, a fuel or electricity). Furtherly, the Price and EF designate the unitary price and the emission factor that are associated to each energy and water utility, respectively. The **Beginning-of-Life** and **End-of-Life** aspects designate concepts that are defined in chapter 6.

Table 3-35. Definition of primary economic and environmental impact reduction viability indicators

Indicator	Definition	Calculation Formula	
Payback time (Years)	It consists in the ratio between the total capital expenditure associated to the WEIS (CAPEX) and the difference between total produced savings (Sav).	$\mathrm{PB\ (Years)} = \dfrac{\mathrm{CAPEX\ (€)}}{\mathrm{Sav\ (€/year)}}$	(3.177)
Absolute equivalent carbon dioxide emission reduction (kton $CO_{2,eq}$/year)	It consists in the absolute difference between total equivalent carbon dioxide emissions in the baseline scenario ($\mathrm{CO_{2,eq\ Baseline}}$) and the improved scenario ($\mathrm{CO_{2,eq\ WEIS}}$).	$\mathrm{Red.\,CO_{2,eq}}\ (\mathrm{kton\ CO_{2,eq}/year}) = (\mathrm{CO_{2,eq\ Baseline}} - \mathrm{CO_{2,eq\ WEIS}})\ (\mathrm{kton\ CO_{2,eq}/year})$	(3.178)

Table 3-36. Definition of Eco-efficiency promotion indicators

Indicator	Definition	Calculation Formula	
Energy use-related indicators			
Specific Fuel Consumption (GJ/ton)	It consists in the ratio between the total consumption of a fuel such as natural gas (FC) and the total quantity of produced material (Prod) in a plant, assessing the dependency of the production process on the use of a determinate fuel.	$\mathrm{SFC\ (GJ/ton)} = \dfrac{\mathrm{FC\ (GJ/year)}}{\mathrm{Prod\ (ton/year)}}$	(3.179)

Specific Electricity Consumption (MWh/ton)	It consists in the ratio between the total consumption of electricity (ElecC) and the total quantity of produced material (Prod) in a plant, assessing the dependency of the production process on the use of electric energy.	$\mathrm{SElecC}\ (\mathrm{MWh/ton}) = \frac{\mathrm{ElecC}\ (\mathrm{MWh/year})}{\mathrm{Prod}\ (\mathrm{ton/year})}$	(3.180)
	Water system-related indicators		
Specific Water Consumption (m^3/ton)	It consists in the ratio between the total consumption of freshwater (FW) and the total quantity of produced material (Prod) in a plant, assessing the dependency of the production process on the use of water resources.	$\mathrm{SFW}\ (\mathrm{m^3/ton}) = \frac{\mathrm{FW}\ (\mathrm{m^3/year})}{\mathrm{Prod}\ (\mathrm{ton/year})}$	(3.181)
Water energy footprint (MJ/m^3)	It consists in the ratio between the energy consumed in the water system (namely the one corresponding to the consumption of hot and cold utilities) (EWS) and freshwater consumption (FW), assessing the dependency of the production process on the use of water resources.	$\mathrm{WEF}\ (\mathrm{MJ/m^3}) = \frac{\mathrm{EWS}\ (\mathrm{MJ/year})}{\mathrm{FW}\ (\mathrm{m^3/year})}$	(3.182)
	GHG emissions-related indicators		
Produced material emission intensity (ton $CO_{2,eq}$/ ton material)	It consists in the ratio between total equivalent carbon dioxide emissions in the plant ($\mathrm{CO_{2,eq}}$) and the quantity of produced material (Prod), assessing the footprint of greenhouse gas emissions on the production process.	$\mathrm{GHGI}\ \left(\mathrm{ton\ CO_{2,eq}/ton\ Prod}\right) = \frac{\mathrm{CO_{2,eq}}\ \left(\mathrm{ton\ CO_{2,eq}/year}\right)}{\mathrm{Prod}\ (\mathrm{ton\ Prod/year})}$	(3.183)
Energy carbon footprint (ton $CO_{2,eq}$/ TJ)	It consists in the ratio between total equivalent carbon dioxide emissions in the plant ($\mathrm{CO_{2,eq}}$) and total energy consumption (EC), assessing the average emission factor associated to the energy mix of the plant.	$\mathrm{EGHGF}\ \left(\mathrm{ton\ CO_{2,eq}/TJ}\right) = \frac{\mathrm{CO_{2,eq}}\ \left(\mathrm{ton\ CO_{2,eq}/year}\right)}{\mathrm{EC}\ (\mathrm{TJ/year})}$	(3.184)
	Aggregated Eco-efficiency indicators		
Aggregated Eco-efficiency indicator (€/kg $CO_{2,eq}$)	It consists in the ratio between the revenue associated to produced material sales ($\mathrm{Revenue}$) and total equivalent carbon dioxide emissions ($\mathrm{CO_{2,eq}}$), assessing the increase of production value in relation to the generated environmental burden.	$\mathrm{EcoEff}\ \left(€/\mathrm{kg\ CO_{2,eq}}\right) = \frac{\mathrm{Revenue}\ (€/\mathrm{year})}{\mathrm{CO_{2,eq}}\ \left(\mathrm{kg\ CO_{2,eq}/year}\right)}$	(3.185)
Produced material productivity (€/kg material)	It consists in the ratio between the revenue associated to produced material sales ($\mathrm{Revenue}$) and total equivalent carbon dioxide emissions ($\mathrm{CO_{2,eq}}$), assessing the increase of production value in relation to the generated environmental burden.	$\mathrm{PMP}\ (€/\mathrm{kg\ Prod}) = \frac{\mathrm{Revenue}\ (€/\mathrm{year})}{\mathrm{Prod}\ (\mathrm{kg\ Prod/year})}$	(3.186)

Table 3-37. Definition of Circular economy promotion indicators

Indicator	Definition	Calculation Formula	
	Energy use-related indicators		
Waste Heat to Total Energy Ratio	It consists in the ratio between waste heat and heat loses (WH) and total energy consumption in the plant (EC).	$\mathrm{WHE} = \frac{\mathrm{WH}\ (\mathrm{TJ/year})}{\mathrm{EC}\ (\mathrm{TJ/year})}$	(3.187)

Recirculated Heat to Baseline Total Energy Ratio	It consists in the ratio between recirculated heat (RH) and total energy consumption in the plant in the baseline scenario ($EC_{Baseline}$).	$\mathrm{RHEB} = \frac{\mathrm{RH}\ (\mathrm{TJ/year})}{\mathrm{EC_{Baseline}}\ (\mathrm{TJ/year})}$	(3.188)
Waste Heat to Fuel Used in Combustion-based Processes Ratio	It consists in the ratio between waste heat from combustion-based processes (WH_{TP}) and respective fuel consumption (FC_{TP}).	$\mathrm{WHFTP} = \frac{\mathrm{WH_{TP}}\ (\mathrm{TJ/year})}{\mathrm{FC_{TP}}\ (\mathrm{TJ/year})}$	(3.189)
Recirculated Heat to Baseline Fuel Used in Combustion-based Processes Ratio	It consists in the ratio recirculated heat in-between combustion-based processes (RH_{TP}) and respective fuel consumption (FC_{TP}).	$\mathrm{RHFTP} = \frac{\mathrm{RH_{TP}}\ (\mathrm{TJ/year})}{\mathrm{FC_{TP}}\ (\mathrm{TJ/year})}$	(3.190)
Water use-related indicators			
Discharge Water to Freshwater Ratio	It consists in the ratio between discharge water from the water system (DW) and freshwater (FW).	$\mathrm{DWFW} = \frac{\mathrm{DW}\ (\mathrm{m^3/year})}{\mathrm{FW}\ (\mathrm{m^3/year})}$	(3.191)
Treated water to Wastewater Ratio	It consists in the ratio between output treated water from wastewater treatment (TW) and input wastewater (WW).	$\mathrm{TWWW} = \frac{\mathrm{TW}\ (\mathrm{m^3/year})}{\mathrm{WW}\ (\mathrm{m^3/year})}$	(3.192)
Recirculated to Produced Treated Water Ratio	It consists in the ratio between recirculated treated water (RTW) and the total produced treated water from wastewater treatment (TW).	$\mathrm{RTWTW} = \frac{\mathrm{RTW}\ (\mathrm{m^3/year})}{\mathrm{TW}\ (\mathrm{m^3/year})}$	(3.193)
Recirculated Treated Water to Water Savings	It consists in the ratio between recirculated treated water (RTW) and the difference between freshwater consumption in the baseline ($FW_{Baseline}$) and improved scenarios (FW_{WEIS}).	$\mathrm{RTWWSav} = \frac{\mathrm{RTW}\ (\mathrm{m^3/year})}{(\mathrm{FW_{Baseline}} - \mathrm{FW_{WEIS}})\ (\mathrm{m^3/year})}$	(3.194)
Energy Input in the Water System-related Indicators			
Energy in Water System in the Improved Scenario over the Baseline Scenario	It consists in the ratio between the energy input in the water system standalone (namely hot and cold utilities and recirculated heat from combustion-based processes) in the improved scenario (EWS_{WEIS}) and the baseline scenario ($EWS_{Baseline}$).	$\mathrm{EWSR} = \frac{\mathrm{EWS_{WEIS}}\ (\mathrm{MJ/year})}{\mathrm{EWS_{Baseline}}\ (\mathrm{MJ/year})}$	(3.195)
Withdrawn Energy from the Water System in the Improved Scenario over Energy in the Water System in the Baseline Scenario	It consists in the ratio between the energy withdrawn from the water system in the improved scenario (namely the difference between total energy input in the water system standalone in the baseline scenario and the total energy input in the improved scenario) (wEWS) and the total energy input in the baseline scenario ($EWS_{Baseline}$).	$\mathrm{wEWEWS} = \frac{\mathrm{wEWS}\ (\mathrm{MJ/year})}{\mathrm{EWS_{Baseline}}\ (\mathrm{MJ/year})}$	(3.196)

Table 3-38. Definition of primary calculation formulas

Aspect	Calculated Formula
Economic savings and equivalent carbon dioxide emission determination	

	$$\begin{aligned}\text{Sav}\ (€/\text{year}) &= (\text{FW}_{\text{Baseline}} - \text{FW}_{\text{WEIS}})\ (\text{m}^3/\text{year}) \cdot \text{Price}_{\text{W}}\ (€/\text{m}^3)\\ &+ \sum_{\text{i}=1} (\text{EC}_{\text{i,Baseline}} - \text{EC}_{\text{i,WEIS}})\ (\text{J}/\text{year}) \cdot \text{Price}_{\text{ES,i}}\ (€/\text{J})\end{aligned}$$	(3.197)
	$$\text{CO}_{2,\text{eq}}\ (\text{kg CO}_{2,\text{eq}}/\text{year}) = \sum_{\text{i}=1} \text{EC}_{\text{i}}\ (\text{J}/\text{year}) \cdot \text{EF}_{\text{ES,i}}\ (\text{kg CO}_{2,\text{eq}}/\text{J}) + \text{Other Emissions}\ (\text{kg CO}_{2,\text{eq}}/\text{year})$$	(3.198)
	Revenue determination	
Beginning-of-Life	$$\text{Revenue}_{\text{WEIS}} = (\text{Revenue}_{\text{Baseline}} + \text{Sav}) - \text{CAPEX}$$	(3.199)
End-of-Life	$$\text{Revenue}_{\text{WEIS}} = (\text{Revenue}_{\text{Baseline}} + \text{Sav})$$	(3.200)

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4. Simulation Models for System-level

In this chapter, several system-level models for Water and Energy Integration Systems (WEIS) to be installed in two sectorial case-study plants are presented. These are set to be developed by assembling several of the previously mentioned component models. For each case-study, it will be presented the model assembling (virtually conceptualization of the WEIS flowsheet), the simulation results (for variables of interest) and the performance of scenario analyses (based on different configurational aspects related to the most general conceptualized WEIS, such as equivalent technologies). In the context of this work, the two characterised case studies set within the Portuguese ceramic sector were selected by attending to the following reasons:

- The representativeness of the ceramic sector within the overall process industry in terms of energy and water use. This sector presents reasonable levels of energy and water use and associated waste streams, and the order of magnitude of the quantity of each resource to be valorised is compatible so as to permit significant savings for each one (for instance, waste heat may be recirculated to cause either significant fuel and electricity savings or to produce a significant level of treated water to be recirculated);
- Both case studies are comparable in terms of the existing energy- and water-using processes (these are based on the same categories of processes) and in terms of the order of magnitude of energy and water consumption;
- Significant availability of data associated with the baseline scenario. The numerical data associated with each parameter of interest characterising the case study are highly discerned (in opposition to similar process industry case studies that are either set in different sectors or in different countries).

4.1. Case-study 1: Standard Configuration

The practical aim of Case-study 1 is to analyse and assess the implementation of a WEIS attending to the standard WEIS configuration (Configuration 1) presented in chapter 3. This case-study is set in a ceramic industry plant (a sanitaryware production facility) located in Portugal. The plant contains combustion-based processes operating in a continuous mode (tunnel kilns), another set of these processes operating in batch production (intermittent kilns) and a set of water-using processes operating in continuous mode. The analysis and assessment procedures taken for this case-study are set to approach the continuous mode processes, namely tunnel kilns and the water-using processes, which are conjointly the ones associated to the most significant use of water and energy.

Plant Characterization and Description

The sanitaryware production plant is constituted by:

- Two tunnel kilns;
- One intermittent kiln;
- Four water-using lines, in its turn constituted by:
    - Four water-using processes, each one installed to remove a specific unidentified salt contaminant;
    - Four heaters, which are hot water boilers using natural gas (as hot utility);
    - One cooler, which is a heat exchanger in which a refrigeration organic fluid (cold utility) stream withdraws enthalpy from the water stream (electricity is used to generate the refrigeration stream through its passage in a cooling tower).

The combustion-based processes (kilns) and the water-using lines' heaters use natural gas as fuel/ hot utility. Currently, there is an interest of the plant stakeholders to reduce total water and energy use (especially natural gas). In Table 4–1, it is presented the complete characterization of the water and energy consumption in the plant. In Figures 4.1 and 4.2, the flowsheets of the considered water system and combustion-based processes are respectively presented.

Table 4-1. Energy and water use data for Case-study 1 Plant

General Data							
Operational Time (h/year)	7824						
Annual Energy Use in the Plant							
Parcel	**Energy Consumption (TJ)**					**Use Share**	
Natural Gas	304.10					81.04%	
Electricity	67.45					17.97%	
Liquified petroleum gas	0.45					0.12%	
Diesel fuel	3.27					0.87%	
Total	375.26						
Natural Gas Consumption in Combustion-based Thermal Processes							
Process	**Energy Consumption (TJ)**					**Use Share**	
Tunnel Kiln 1	69.34					18.48%	
Tunnel Kiln 2	36.52					9.73%	
Annual Energy and Water Consumption in Water-using Lines							
Water-using Line	**Water Consumption (dam^3)**		**Heater Hot Utility Consumption (TJ)**	**Use Share**		**Cooler Cold Utility Consumption (TJ)**	**Use Share**
Line 1	3.72		1.37	0.37%			
Line 2	3.73		1.43	0.38%			
Line 3	2.86		1.04	0.28%			
Line 4	0.46		0.18	0.05%			
Discharge Line						4.52	1.20%
Total	10.77		4.01	1.07%		4.52	1.20%

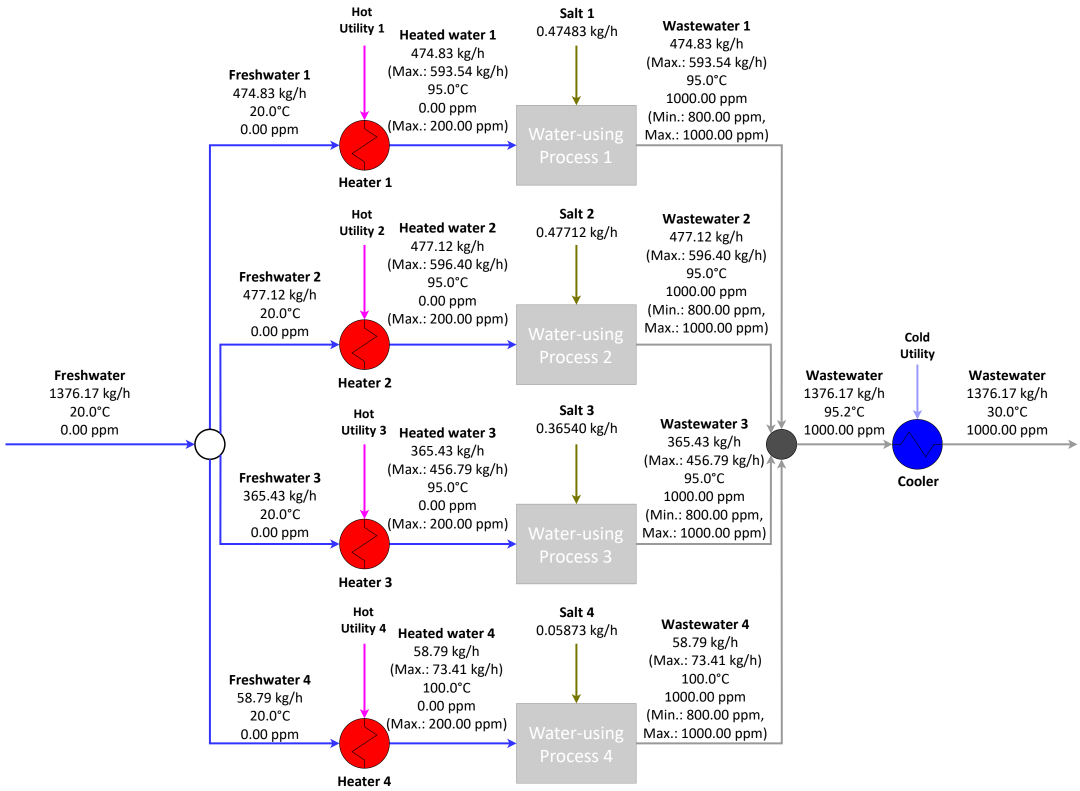
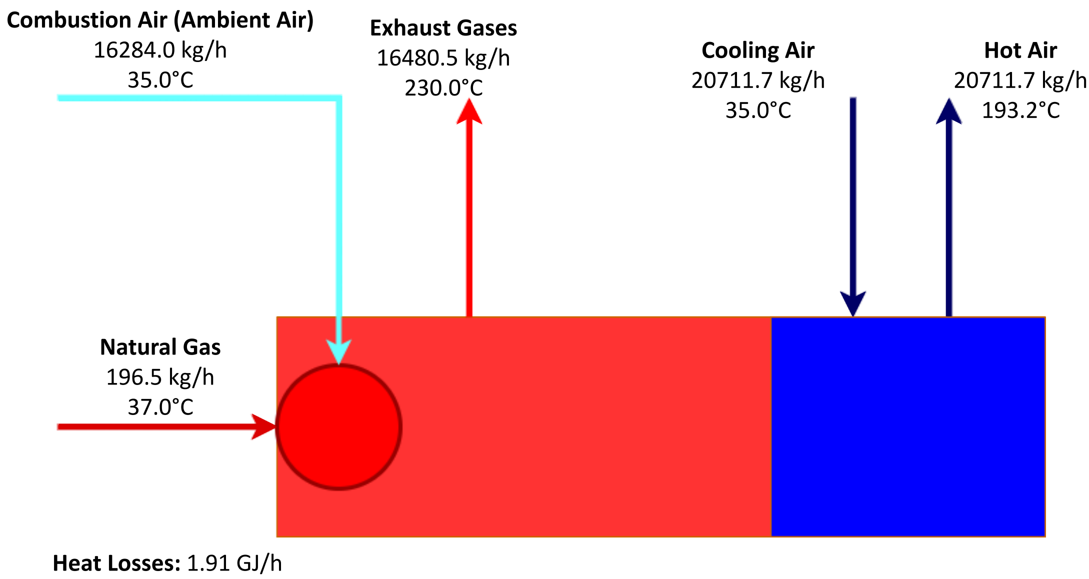
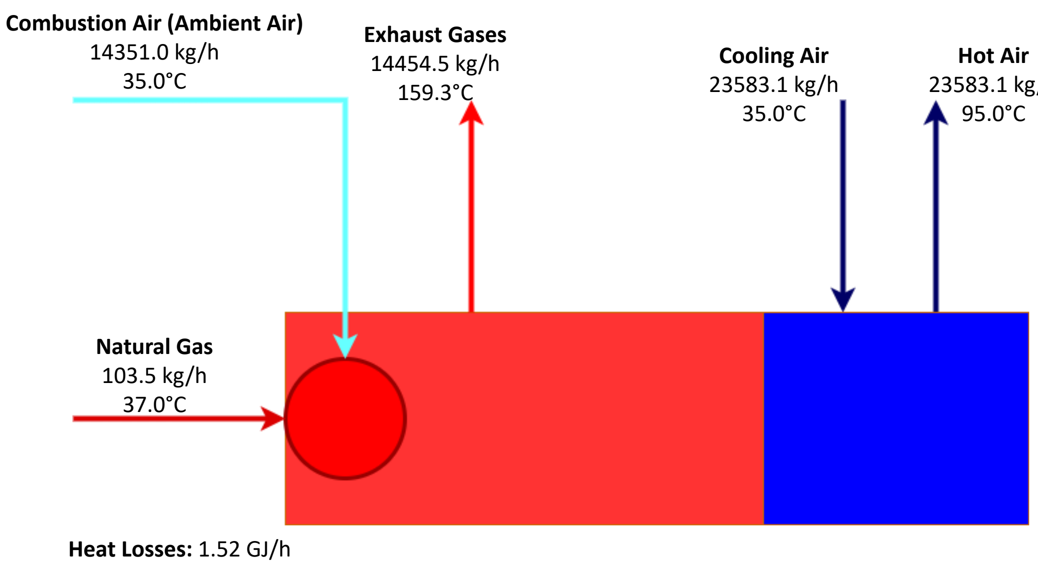


Figure 4.1. Flowsheets of the water-using lines including stream data (mass flow rates, temperatures, salt contaminant concentrations), including minimum and maximum values (Case-study 1)



a)



b)

Figure 4.2. Flowsheets of Tunnel Kilns including stream data (mass flow rate and temperatures) and heat losses (Case-study 1): a) Tunnel Kiln 1, b) Tunnel Kiln 2

As may be verified by the analysis of Table 4–1, the most significant parcel of energy use in the case-study plant is natural gas used as fuel. Within the total natural gas consumption, it is to highlight the significant contribution of the two tunnel kilns, which conjointly represent 28.21% of the total energy consumption in the industrial site. The electricity use follows as the second most significant parcel. In its turn, liquified petroleum gas and diesel fuel represent only minor parcels of the total energy use. In relation to the water system (comprising all water-using lines), it is possible to verify that the total hot utility consumption represents 1.07% of the total energy consumption, while the cold utilities consumption represents 1.20%. These values are significant of a relatively high representativity of the energy input on the water system in relation to the total energy consumption (taking into account the common misconception that the energy use in water systems may be considered negligible).

In the scope of heat recovery system conceptualization, the outlet streams from the tunnel kiln represented in Figure 4.2 that may be considered for waste heat valorisation are both the exhaust gases streams and the hot air streams. Since the exhaust gases are the ones resulting from combustion, these contain a determinate share of components (such as CO_2 and NO_x). The presence of such components may limit the temperature withdrawal of the exhaust gases streams (achieved by heat transfer from the recirculated heat stream to the heat sink) to a determinate dew point temperature, in which there is a risk of condensation of the gas. Such constraint must be imposed to avoid the risk of corrosion of industrial equipment.

System Retrofitting Approaches

Taking into account the data presented for the characterization of the existing energy and water-using processes, it is possible to formulate several system retrofitting approaches based on the adaption of the general WEIS Configuration 1 to this case-study. In Table 4-2, it is presented the characterization of three conceptualized WEIS scenarios for the present case-study. The flowsheets corresponding to each one of these scenarios (respectively designated Scenario 1 and 2) are presented in Figures 4.3 and 4.4.

Table 4-2. Characterization of conceptualized Scenarios

Scenario	Characterization
1	• The general flowsheet results from the adaption of the Standard WEIS Configuration (Configuration 1) considering 2 combustion-based processes (the two tunnel kilns installed in the plant) and 4 water-using processes (which are the water-using processes installed in each water-using lines); • Each one of the two kilns is characterized by having two waste heat streams: exhaust gas streams and hot air streams; • The considered TC technology is an Organic Rankine cycle (ORC); • The considered WWT technology is a Multi-effect distillation (MED) unit; • The considered WWtE technology is an Electrolysis unit; • While the hot air stream is set to be recirculated between the two tunnel kilns and the MED unit, the exhaust gas streams are set to be recirculated to the ORC; • The hot air stream at the outlet of the MED unit is then recirculated to be mixed with the conjoined exhaust gas streams, then the mixed gas stream recirculated to the ORC; • The hydrogen produced in the Electrolysis unit is then distributed to the fuel inlet of each one of the tunnel kilns so to produce hydrogen-enriched natural gas (HENG).
2	• The general flowsheet results from the adaption of the Standard WEIS Configuration (Configuration 1), being generally the same as the one from Scenario 1 considering the configurational changes described below; • The exhaust gas streams from each tunnel kiln are transported to two air-gas heat exchangers (air preheaters) to exchange heat with the two combustion air streams; • The two hot air streams are mixed and recirculated to the ORC and the MED unit.

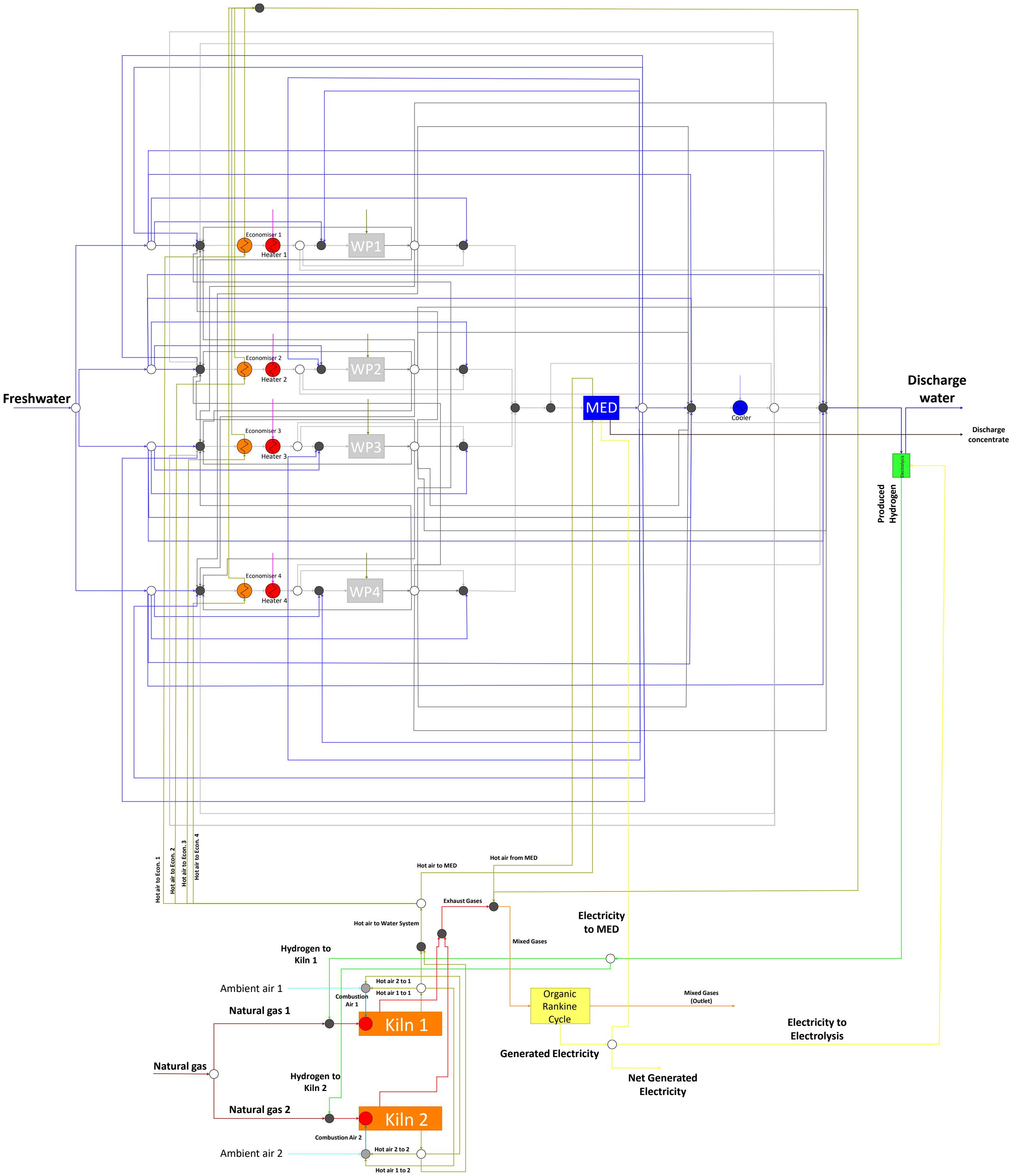


Figure 4.3. Flowsheet assembling of Scenario 1

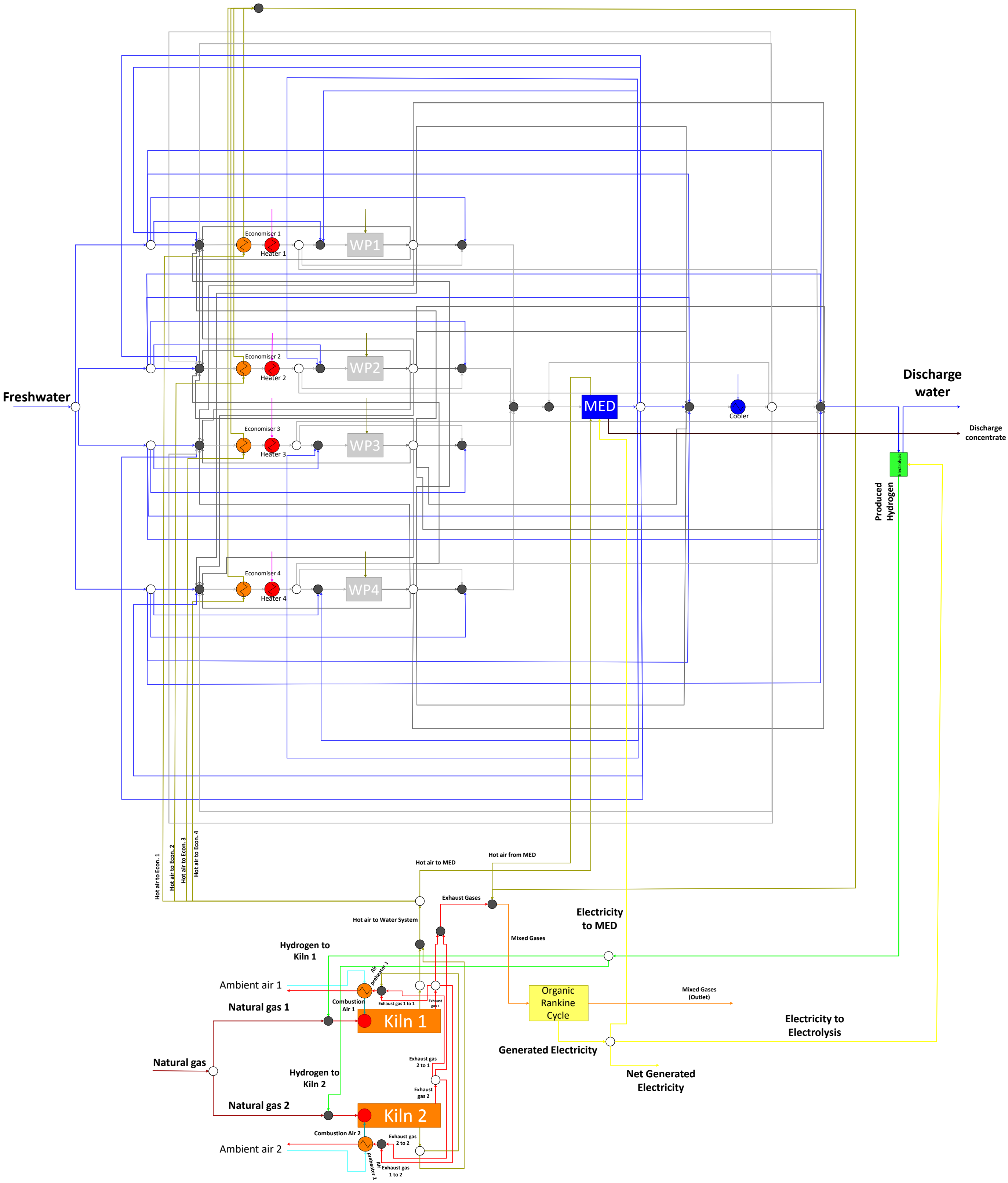


Figure 4.4. Flowsheet assembling of Scenario 2

Model Assembling

The definition of the two scenarios in the previous section serves as the starting point for the assembling of system-level models using the capabilities of the ThermWatt Modelica library. For the baseline scenario (in which heat recovery or water recirculation has still to be planned) and for each one of the conceptualized scenarios, a simulation model is set to be assembled for the purpose of obtaining simulation results that virtually characterize the thermal, hydraulic and reaction-based phenomena that characterize the industrial systems using the components present in the ThermWatt library. In Figure 4.5, the baseline scenario Modelica model flowsheet is presented. The Scenario 1 and 2 model flowsheets are presented in Figures 4.6 and 4.7, respectively. The setup of specific parameters associated to equipment sizing and operational details associated to the conceptualized structure are presented in Table 4-3. The properties associated to the considered working fluids and media are characterized in appendix A4.

Table 4-3. Setup of specific parameters and operational details associated to the components models of case-study 1

Component		
Multi-effect distillation (MED)		• The unit is constituted by five effects and one condenser; • The whole quantity of the wastewater stream enters the condenser and it is then equally distributed into the five effects; • The heat transfer area parameter associated to the first effect is set to the value of 1 m^2; • The overall heat transfer coefficient associated to the first effect is set to the value of 400 W/(m^2.ºC).
Organic Rankine Cycle (ORC)	General	• The considered working fluid is NOVEC649.
	Centrifugal pump	• The outlet pressure is set at the value of 7 bar.
	Regenerator	• The pressure loss (liquid side) is set at the value of 4 bar; • The heat transfer efficiency associated to the regenerator is set at the value of 100%; • The overall heat transfer coefficient is set at the value of 400 W/(m^2.ºC); • The outlet temperature of the liquid stream is set at the value of 52 ºC (which is the boiling point temperature associated to the NOVEC649 fluid).
	HRSG Unit	• The overall heat transfer coefficient associated to the superheater within the HRSG unit is set at the value of 70 W/(m^2.ºC); • The outlet temperature of the hot stream (mixed gas stream) is set at 75 ºC (dew point temperature set for the mixed gas stream).
	Vapour Turbine	• The mechanical efficiency associated is set at the value of 85.0%; • The hydraulic efficiency associated is set at the value of 80.0%.
Air preheaters		• The overall heat transfer coefficient is set at the value of 70 W/(m^2.ºC).
Electrolysis		• The electricity-to-hydrogen conversion rate is set at the value of 70.0%.

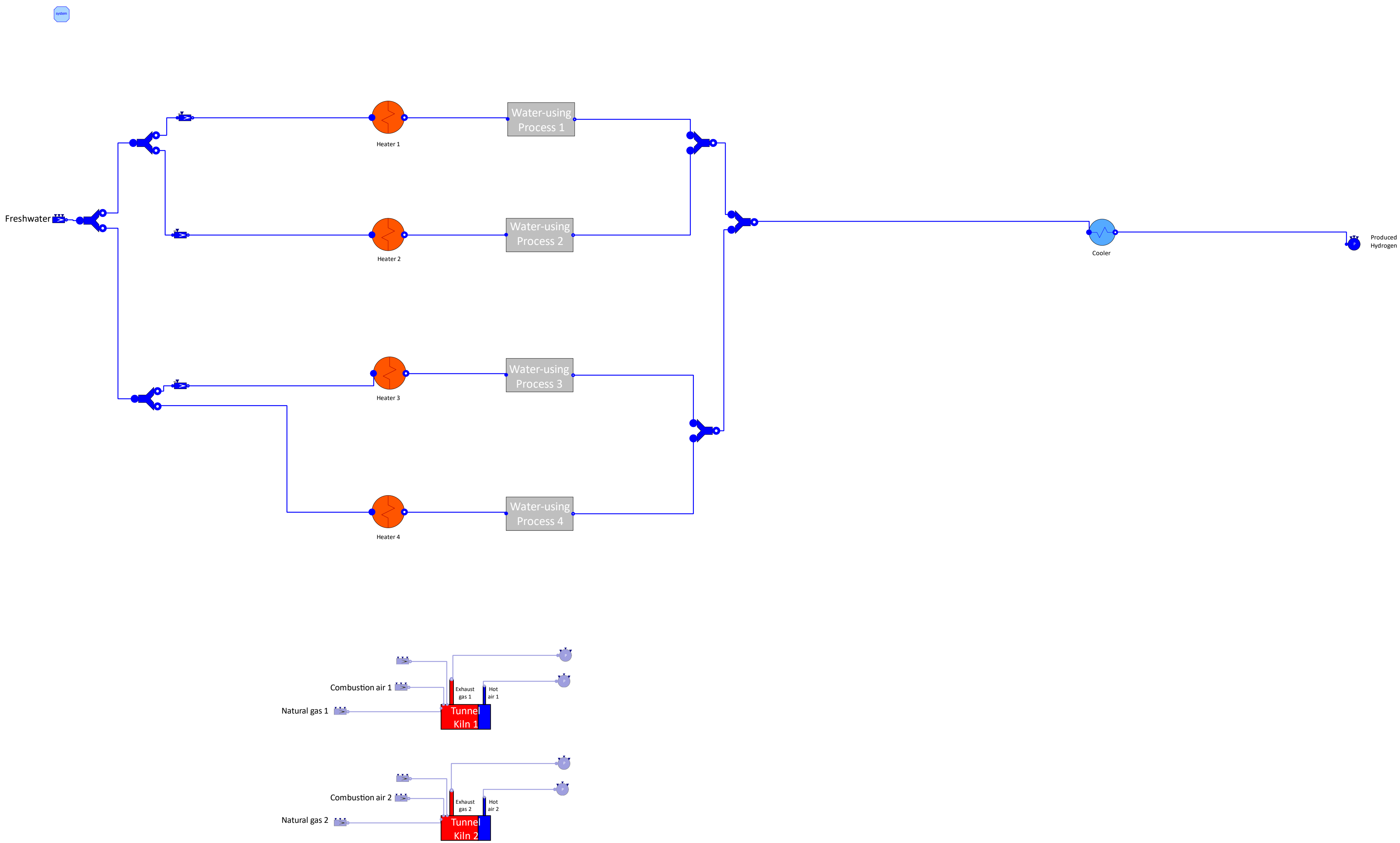


Figure 4.5. Flowsheet assembling of Baseline Scenario using the ThermWatt Modelica library capabilities

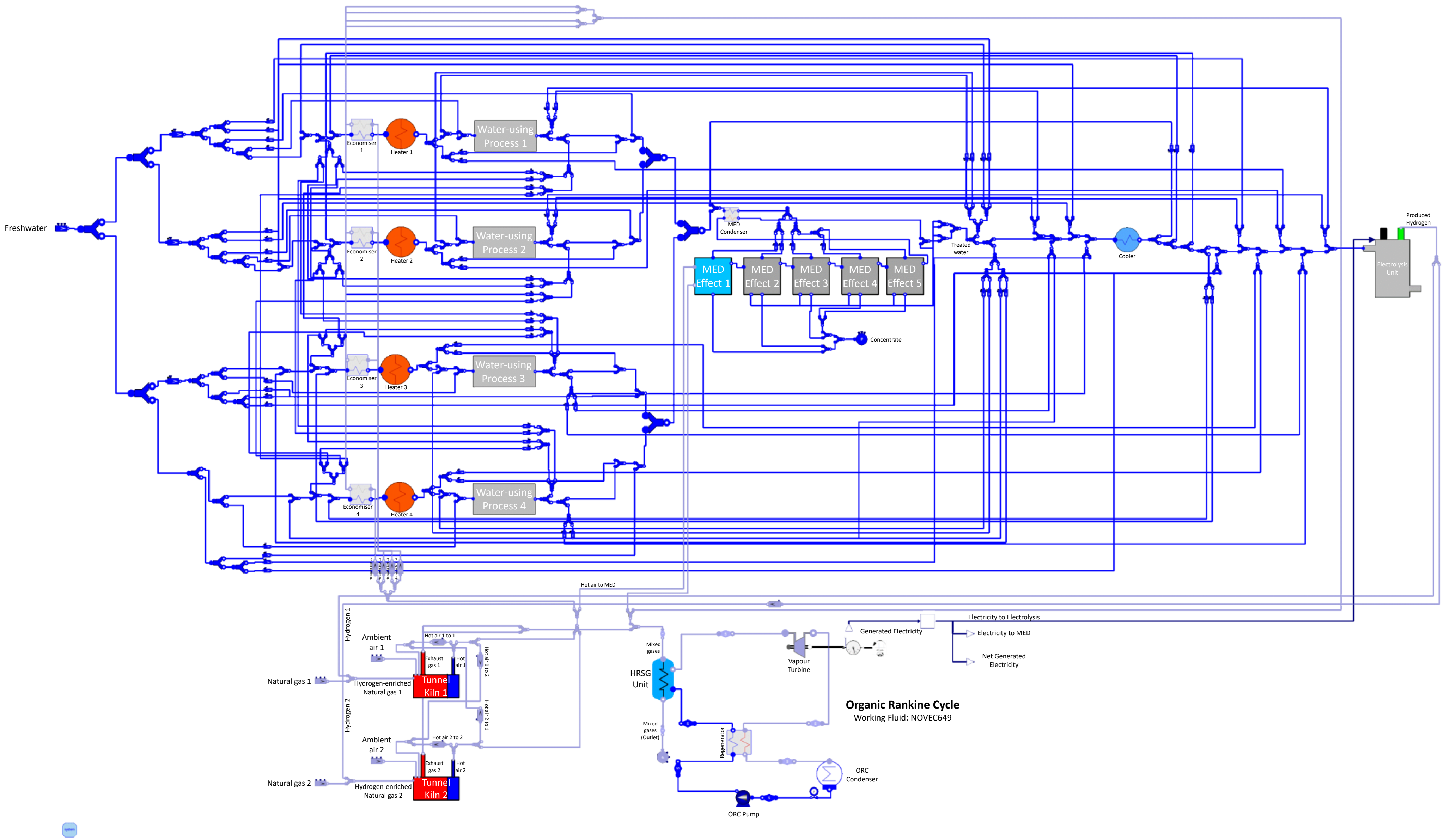


Figure 4.6. Flowsheet assembling of Scenario 1 using the ThermWatt Modelica library capabilities

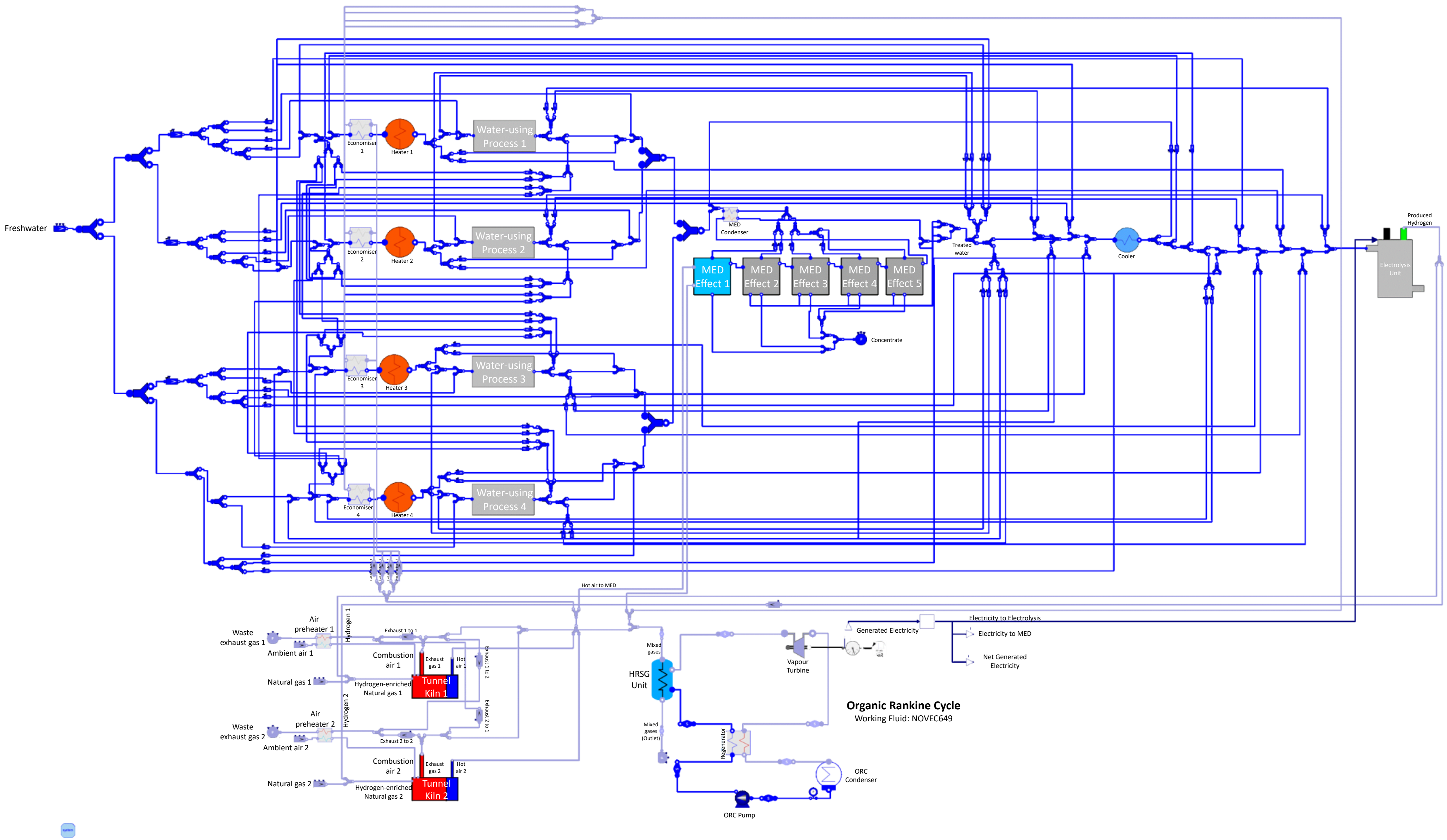


Figure 4.7. Flowsheet assembling of Scenario 2 using the ThermWatt Modelica library capabilities

Scenario Analysis

The conceptualized scenarios 1 and 2 are set to be compared with the aim to assess which scenario has the highest potential in terms of the reduction of total cost. A set of parameters related to stream recirculation was considered common for both scenarios, with the aim to establish a basis of comparison. Therefore, the following parameters were set as constant in-between both scenarios:

- The temperature of the combustion air at the inlet of tunnel kilns 1 and 2 was set as 153.19ºC and 81.52ºC, respectively;
- The mass flow rate of each one of the four hot air streams allocated to the air-gas heat exchangers installed in the water system was set as 3000 kg/h;
- The mass flow rate of the hot air streams recirculated to the air-gas heat exchangers were set to allow the hot utility consumption on the heaters of the water system to be null;
- The mass flow rate of the treated water stream that is not recirculated from the outlet of the MED unit was set as null, to allow for the cold utility consumption in the water system cooler to be null as well;
- The mass flow rate of the recirculated treated water from the outlet of the MED unit to the inlet of the heater in water-using line 4 was set as 58.79 kg/h, with the remaining quantity of treated water being equally distributed to each one of the of the remaining three water-using lines;
- For the hydrogen production cases, a quantity of 58.79 kg/h of the outlet water stream from the water system is considered. Such corresponds to the quantity of water stream that would be recirculated to the inlet of water-using process 4, and in this case it is instead directed to the Electrolysis unit.

In Table 4-4, the simulation results for each one of the scenarios are presented. Two sub-scenarios were considered for both scenario 1 and 2, namely one considering that all the electricity produced on the ORC is furtherly used for electricity savings and the other considering that all produced electricity is used on the Electrolysis unit for hydrogen production.

Table 4-4. Results for the scenario analysis of Case-study 1

Utility/ Cost Parcel		Baseline	Scenario 1		Scenario 2	
			With Electricity Production	With Hydrogen Production	With Electricity Production	With Hydrogen Production
Thermal Process System						
Natural Gas Flow Rate (kg/h)	Tunnel Kiln 1	196.5	160.38	156.56	160.38	156.52
	Tunnel Kiln 2	103.5	90.21	90.21	90.21	90.21
Net Generated Electricity (kWh/h)			91.66		89.89	
Water System						
Freshwater Flow Rate (kg/h)		1376.17	935.75	994.54	910.40	969.82

Overall						
Total Operational Cost (€/h)	350.88	255.75	265.16		255.97	265.07
Total Operational Cost (M€/year)	2.75	2.00	2.07		2.00	2.07

The total operational cost indicators considered in Table 4-4 were calculated by the summation of the costs associated to each energy parcel and freshwater, based on unitary values for the Portuguese industrial sector associated to each one of the considered parcels:

- 23.66 €/GJ for natural gas [378];
- 0.1459 €/kWh for electricity [379];
- 1.8499 €/m^3 for freshwater [380].

The potential for total cost reduction (which being directly proportional to energy and water use reduction do also effectively convey eco-efficiency promotion) may be compared in-between scenarios through the comparison of the energy and water utilities consumption (namely mass flow rates in kg/h units) and cost parcels (in €/h units). In the widest perspective of the economic evaluation to the WEIS, the total installation cost corresponds to the summation of all the investment cost and operational costs parcels. The comparison between scenarios in the present analysis is primarily performed on the basis of the calculated total operational costs, although aspects related to investment costs for technology installation are also set to be considered in the case that similar results for the total operational costs are obtained. As may be verified by the analysis of Table 4-4, Scenario 1 is the one with the highest cost reduction and therefore eco-efficiency promotion potential. It is possible to perform the even further verifications:

- The installation of water-gas heat exchangers replacing hot air recirculation conducts in Scenario 2 does not produce overall benefits in comparison to WEIS configuration of Scenario 1;
- In the follow-up of the previous, the highest availability of hot air to be used for electricity production in the ORC does not compensate the exhaust gas quantity that is not used for such purpose and is instead used for natural gas savings in the tunnel kilns;
- With the only benefit that would otherwise be associated to Scenario 2 being not verified (as described in the previous two points), it is added the fact that heat exchanger installation (Scenario 2) is in principle associated to a highest investment cost in comparison duct installation (Scenario 1);
- The relatively lower natural gas consumption levels in Scenario 1 comparatively to Scenario 2 effectively compensate for the respectively higher water consumption (which may be essentially attributed the significantly superior unitary costs of natural gas compared to freshwater);
- For both Scenarios 1 and 2, the case of the use of generated electricity as a direct use for electric energy savings in the plant instead of its use on the Electrolysis unit for hydrogen production compensates in terms of total operation costs savings.

4.2. Case-study 2: Dynamic-based Configuration

The conceptualization of Case-study 2 focus on the analysis of an overall transient mode of operation of the case-study plant, considering the implementation of the dynamic configuration (Configuration 2) presented in chapter 3. As detailed earlier, such WEIS configuration is based on the installation of a thermal energy storage (TES) module to which it is supplied all the existing waste heat streams from the plant and from which the stored heat is then distributed to all the energy-using units. This case-study plant is inserted in a sanitaryware production ceramic industry plant, which is geographically set within the same industrial site as the plant analysed in Case-study 1. The plant is constituted by a set of combustion-based processes operating in a continuous mode (tunnel kilns), another set of these processes operating in batch production (intermittent kilns) and a set of water-using processes operating in a continuous mode.

Plant Characterization and Description

The sanitaryware production plant is constituted by:

- Two tunnel kilns;
- Two intermittent kilns;
- Three water-using lines, in its turn constituted by:
  - Three water-using processes, each one installed to remove a set of three unidentified salt contaminants;
  - Three heaters, which are hot water boilers using natural gas (as hot utility);
  - Three coolers, which are heat exchangers in which refrigeration organic fluid (cold utility) streams withdraws enthalpy from the water stream (electricity is used to generate the refrigeration streams through its passage in a cooling tower).

The combustion-based processes (kilns) and the water-using lines' heaters use natural gas as fuel/ hot utility. Currently, there is an interest of the plant stakeholders to reduce total water and energy use (particularly natural gas). In Table 4-5, it is presented the complete characterization of the water and energy consumption in the plant.

Table 4-5. Energy and water use data for Case-study 2 Plant

General Data		
Operational Time (h/year)	7824	
Annual Energy Utilities Use		
Parcel	**Energy Consumption (TJ)**	**Use Share**
Natural Gas	304.10	81.04%
Electricity	67.45	17.97%
Liquified petroleum gas	0.45	0.12%
Diesel fuel	3.27	0.87%

Total	375.26	
Natural Gas Consumption in Combustion-based Processes		
Tunnel Kilns		
Process	**Energy Consumption (TJ)**	**Use Share**
Kiln 1	44.99	11.99%
Kiln 2	42.38	11.29%

Intermittent Kilns				
Process	**Operation Cycle**		**Energy Consumption (TJ)**	**Use Share**
	Firing Time (Hours)	**Cooling Time (Hours)**		
Kiln 3	16.5	25.5	4.34	1.16%
Kiln 4			16.26	4.33%

Annual Energy and Water Consumption in Water-using Lines					
Water-using Line	**Water Consumption (dam^3)**	**Heater Hot Utility Consumption (TJ)**	**Use Share**	**Cooler Cold Utility Consumption (TJ)**	**Use Share**
Line 1	2.44	0.98	0.26%	0.66	0.18%
Line 2	3.80	1.41	0.38%	1.04	0.28%
Line 3	0.49	0.26	0.07%	0.13	0.04%
Total	6.73	2.65	0.71%	1.84	0.49%

As may be verified by the analysis of Table 4-5, the total natural gas consumption in the four kilns of this plant represent 28.77% of the total energy consumption in the industrial site, with the intermittent kilns representing 23.58% of this parcel. Such constitutes a significant level of energy consumption, attending to the non-continuous character of the operation of these combustion-based processes. The water system is also associated to a considerable energy use, with the associated hot and cold utilities representing 0.71% and 0.49% of the total energy consumption, respectively. In Figures 4.8 and 4.9, the flowsheets of the considered water system and combustion-based processes are respectively presented.

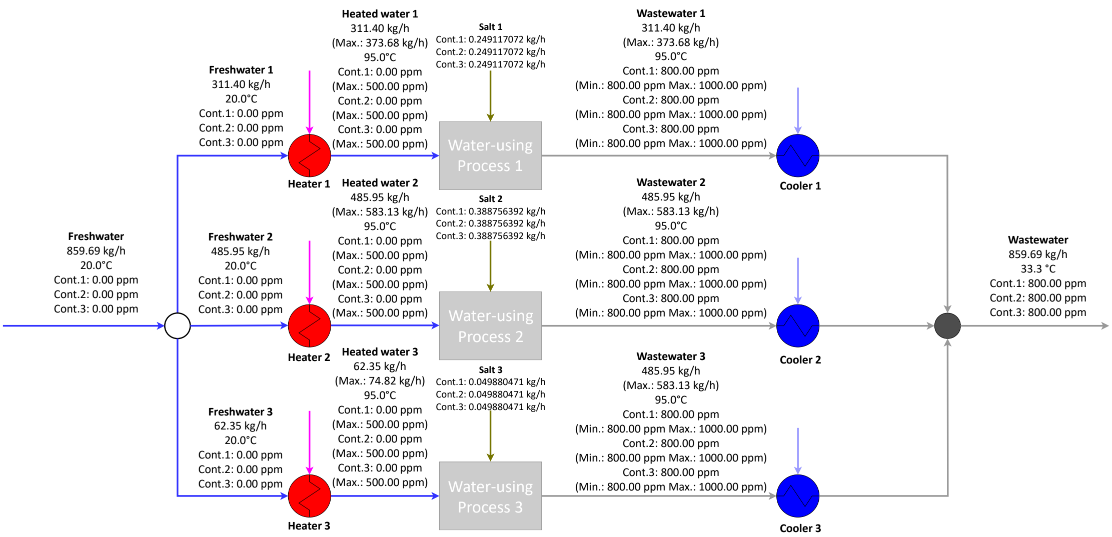
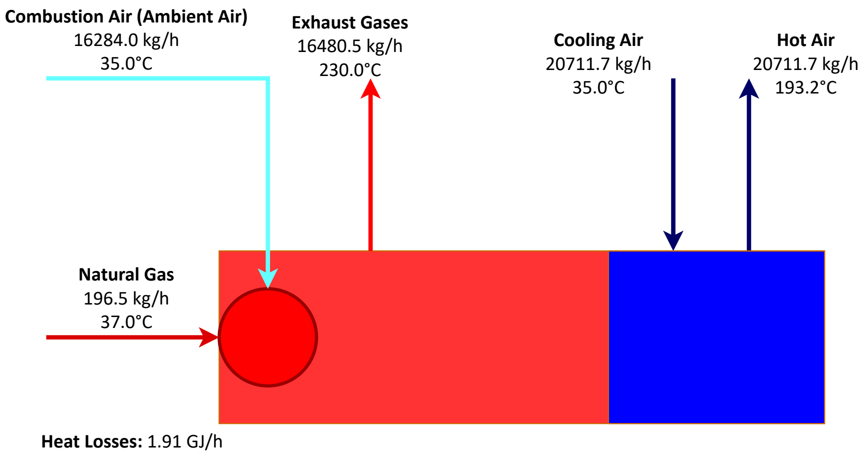
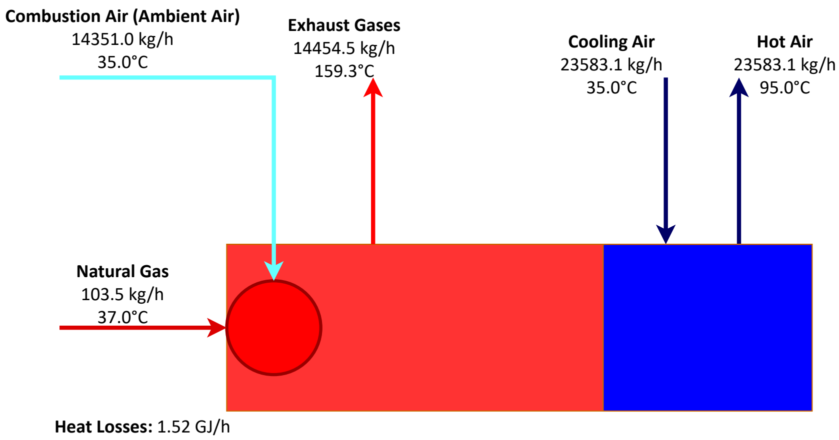


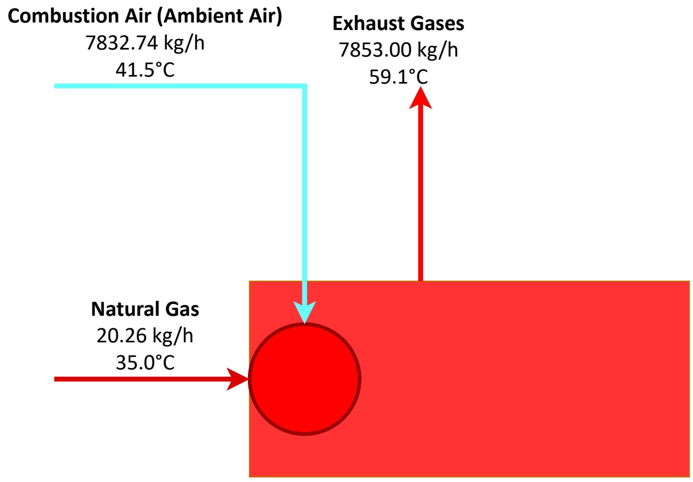
Figure 4.8. Flowsheets of the water-using lines including stream data (mass flow rates, temperatures, salt contaminant concentrations), including minimum and maximum values (Case-study 2)


Combustion Air (Ambient Air)
16284.0 kg/h
35.0°C
Exhaust Gases
16480.5 kg/h
230.0°C
Cooling Air
20711.7 kg/h
35.0°C
Hot Air
20711.7 kg/h
193.2°C
Natural Gas
196.5 kg/h
37.0°C
Heat Losses: 1.91 GJ/h

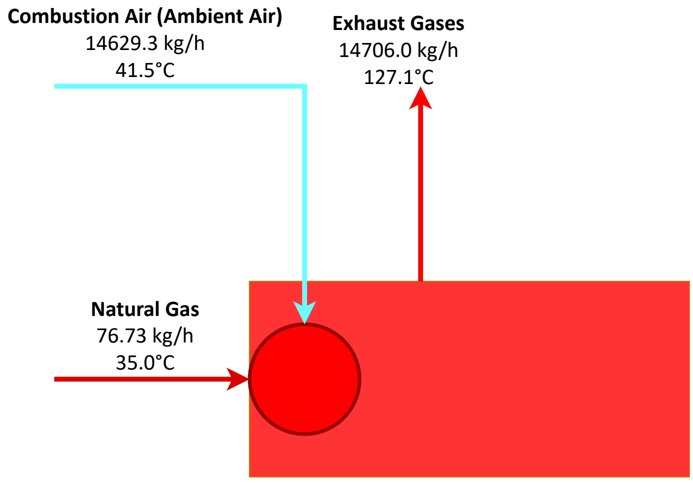
a)


Combustion Air (Ambient Air)
14351.0 kg/h
35.0°C
Exhaust Gases
14454.5 kg/h
159.3°C
Cooling Air
23583.1 kg/h
35.0°C
Hot Air
23583.1 kg/h
95.0°C
Natural Gas
103.5 kg/h
37.0°C
Heat Losses: 1.52 GJ/h

b)


Combustion Air (Ambient Air)
7832.74 kg/h
41.5°C
Exhaust Gases
7853.00 kg/h
59.1°C
Natural Gas
20.26 kg/h
35.0°C

c)



d)

Figure 4.9. Flowsheets of Tunnel Kilns and Intermittent Kilns including stream data (mass flow rate and temperatures) and heat losses (Case-study 2): a) Kiln 1, b) Kiln 2, c) Kiln 3, d) Kiln 4

Similarly to the aforementioned limit conditions of case-study 1, this case-study has also associated constraints at the level of the enthalpy withdrawal from exhaust gases, in which a determinate dew point temperature of the gases must not be surpassed. In addition, the water system constituent of this case-study is also set for the removal of more than one type of solid contaminant (it constitutes a multi-contaminant problem). As such, the simulation model (and by extension the furtherly developed optimisation model counterpart) takes into account the entrance in the system of each of the three mentioned contaminants, as well as the minimum and maximum values of concentration of each water stream.

System Retrofitting Approaches

Taking into account the data presented for the characterization of the existing energy and water-using processes, it is possible to formulate several system retrofitting approaches based on the adaption of the general WEIS Configuration 2 to this case-study. In Table 4-6, it is presented the characterization of three conceptualized WEIS scenarios for the present case-study. The flowsheets corresponding to each one of these scenarios are presented in Figures 4.10 and 4.11 for respectively Scenario 1 and 2.

Table 4-6. Characterization of conceptualized scenarios

Scenario	Characterization
1	• The general flowsheet results from the adaption of the Storage-based WEIS Configuration (Configuration 2) considering 4 combustion-based processes (which are the two tunnel kilns and two intermittent kilns installed in the plant) and 3 water-using processes (which are the water-using processes installed in each water-using lines); • Each one of the two kilns is characterized by having two waste heat streams: exhaust gas streams and hot air streams;

	• The considered TC technology is an Organic Rankine cycle (ORC); • The considered WWT technology is a MED unit; • The considered WWtE technology is an Electrolysis unit; • The considered TES technology is a PCM-based heat exchanger; • During the cooling cycle of the kilns (which is set as the charge time for the storage of enthalpy within the PCM-TES unit), a part of the whole exhaust gas streams from each one of the tunnel kilns is recirculated to the TES unit; • During the firing cycle of the kilns (which is set as the discharge time for the withdrawal of enthalpy from the PCM-TES unit), the aforementioned quantity of exhaust gases is recirculated to the ORC system. • The hot air streams from each one of the two tunnel kilns are recirculated to the respective tunnel kiln and to the HRSG unit of the ORC; • The remaining quantities of the hot air streams from each one of the two tunnel kilns are mixed and recirculated to three water-gas heat exchangers (economisers) installed to heat up the inlet water stream at each one of the water system's heaters and the first effect of the MED unit; • The hot air streams at the outlet of the water-gas heat exchangers and the MED unit are then conjoined and furtherly recirculated to be mixed with the conjoined exhaust gas streams, so then the mixed gas stream to be recirculated to the ORC; • The hydrogen produced in the Electrolysis unit is then distributed to the fuel inlet of each one of the tunnel kilns so to produce hydrogen-enriched natural gas (HENG).
2	• The general flowsheet results from the adaption of the Storage-based WEIS Configuration (Configuration 2), being generally the same as the one from Scenario 1 considering the configurational alterations described below; • A part of the whole hot air streams from each one of the tunnel kilns is recirculated to the TES unit (instead of the exhaust gas streams); • During the cooling cycle of the kilns, a part of the whole hot air streams from each one of the tunnel kilns is recirculated to the TES unit (instead of the exhaust gases); • During the firing cycle of the kilns, the aforementioned quantity of hot air is recirculated to the ORC system.

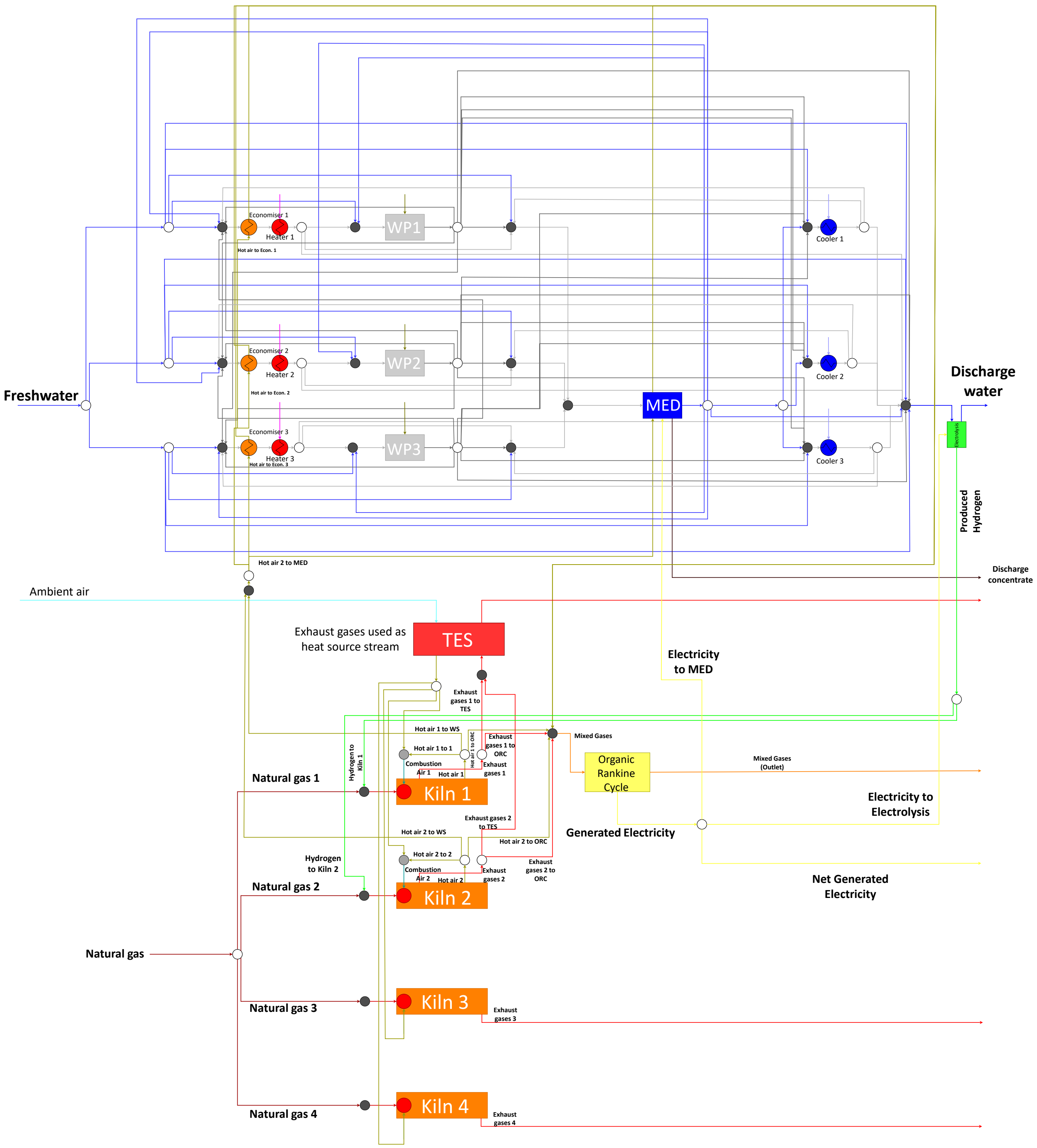


Figure 4.10. Flowsheet assembling of Scenario 1

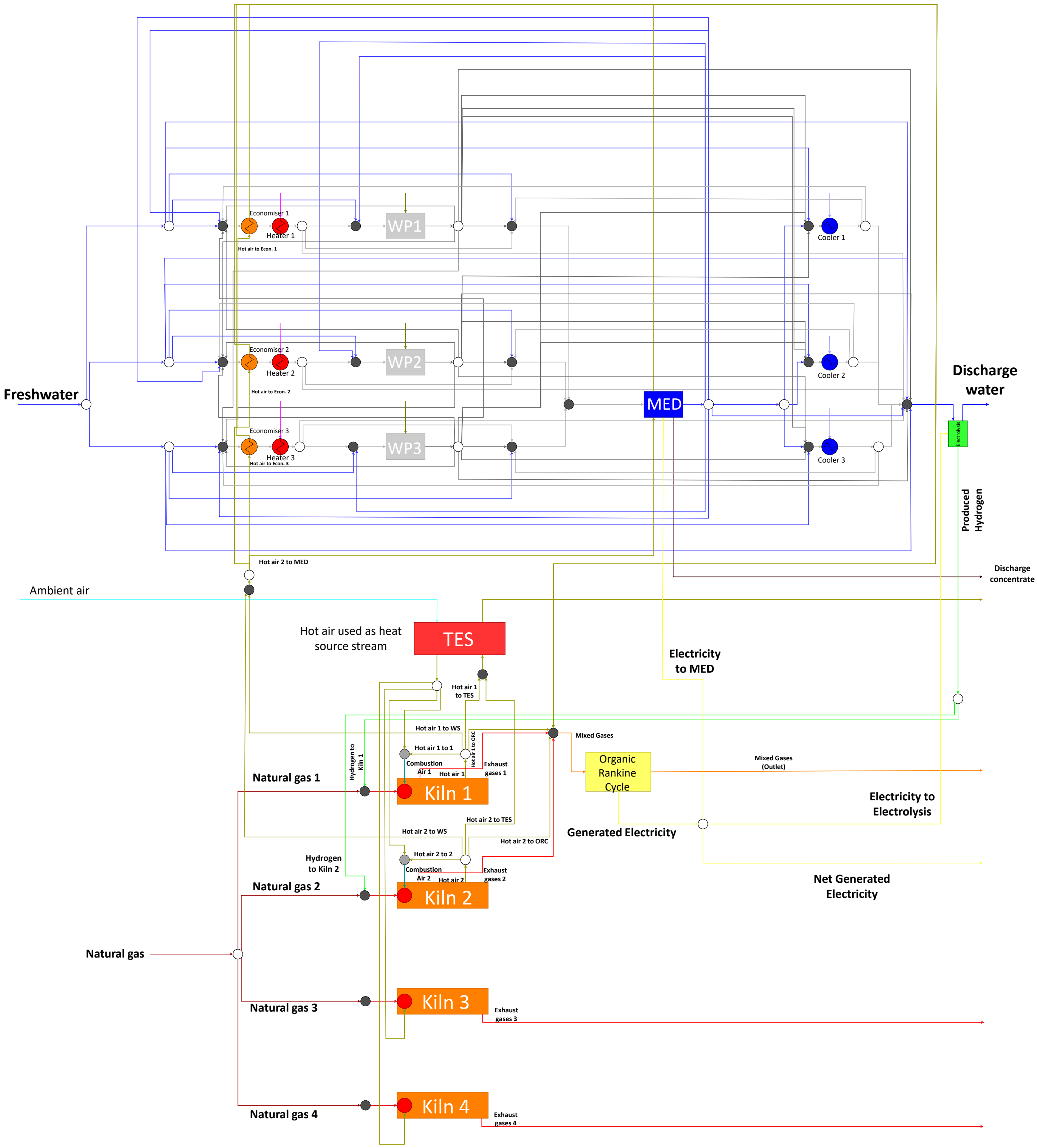


Figure 4.11. Flowsheet assembling of Scenario 2

Model Assembling

The two scenarios presented in the previous section are the basis for the assembling system-level models using the capabilities of the ThermWatt Modelica library. As mentioned afore, the aim of this case-study is the analysis of the changes of certain system variables along with a certain time period (in this case, 42 hours). As such, the developed model is set for dynamic simulation and accounts for a transient state analysis. In Figure 4.12, the baseline scenario Modelica model flowsheet is presented. The Scenario 1 and 2 model flowsheets are presented in Figures 4.13 and 4.14, respectively. The setup of specific parameters associated to equipment sizing and operational details associated to the conceptualized installation are presented in Table 4-7. The properties associated to the considered working fluids and media are characterized in appendix A4.

Table 4-7. Setup of specific parameters and operational details for the component models of case-study 2

Component		Characterization
Multi-effect distillation (MED)		• The unit contains four effects and one condenser; • The whole quantity of the wastewater stream enters the condenser and it is then equally distributed into the four effects; • The heat transfer area parameter associated to the first effect is set to the value of 1.79 m^2; • The overall heat transfer coefficient associated to the first effect is set to the value of 400 W/(m^2.ºC).
Organic Rankine Cycle (ORC)	General	• The considered working fluid is NOVEC649.
	Centrifugal pump	• The outlet pressure is set at the value of 6 bar.
	Regenerator	• The pressure loss (liquid side) is set at the value of 4 bar; • The heat transfer efficiency associated to the regenerator is set at the value of 100%; • The overall heat transfer coefficient is set at the value of 400 W/(m^2.ºC); • The outlet temperature of the liquid stream is set at the value of 52 ºC (which is the boiling point temperature associated to the NOVEC649 fluid).
	HRSG Unit	• The overall heat transfer coefficient associated to the superheater within the HRSG unit is set at the value of 70 W/(m^2.ºC); • The outlet temperature of the hot stream (mixed gas stream) is set at 70 ºC (dew point temperature set for the mixed gas stream).
	Vapour Turbine	• The mechanical efficiency associated is set at the value of 85.0%; • The hydraulic efficiency associated is set at the value of 80.0%.
PCM-based heat exchanger		• The considered phase change material is the commercial material PlusICE Organic Range A73, whose properties are defined in appendix A4. • The number of tubes for the passage of the hot stream is set at the value of 120; • The internal radius parameter associated to the tubes is set at 0.100 m; • The external radius parameter associated to the tubes is set at 0.120 m; • The length parameter associated to the tubes is set at 10.00 m; • The number of nodes for the axial direction is set at the value of 10; • The number of nodes for the radial direction is set at the value of 5.
Electrolysis		• The electricity-to-hydrogen conversion rate is set at the value of 70.0%.

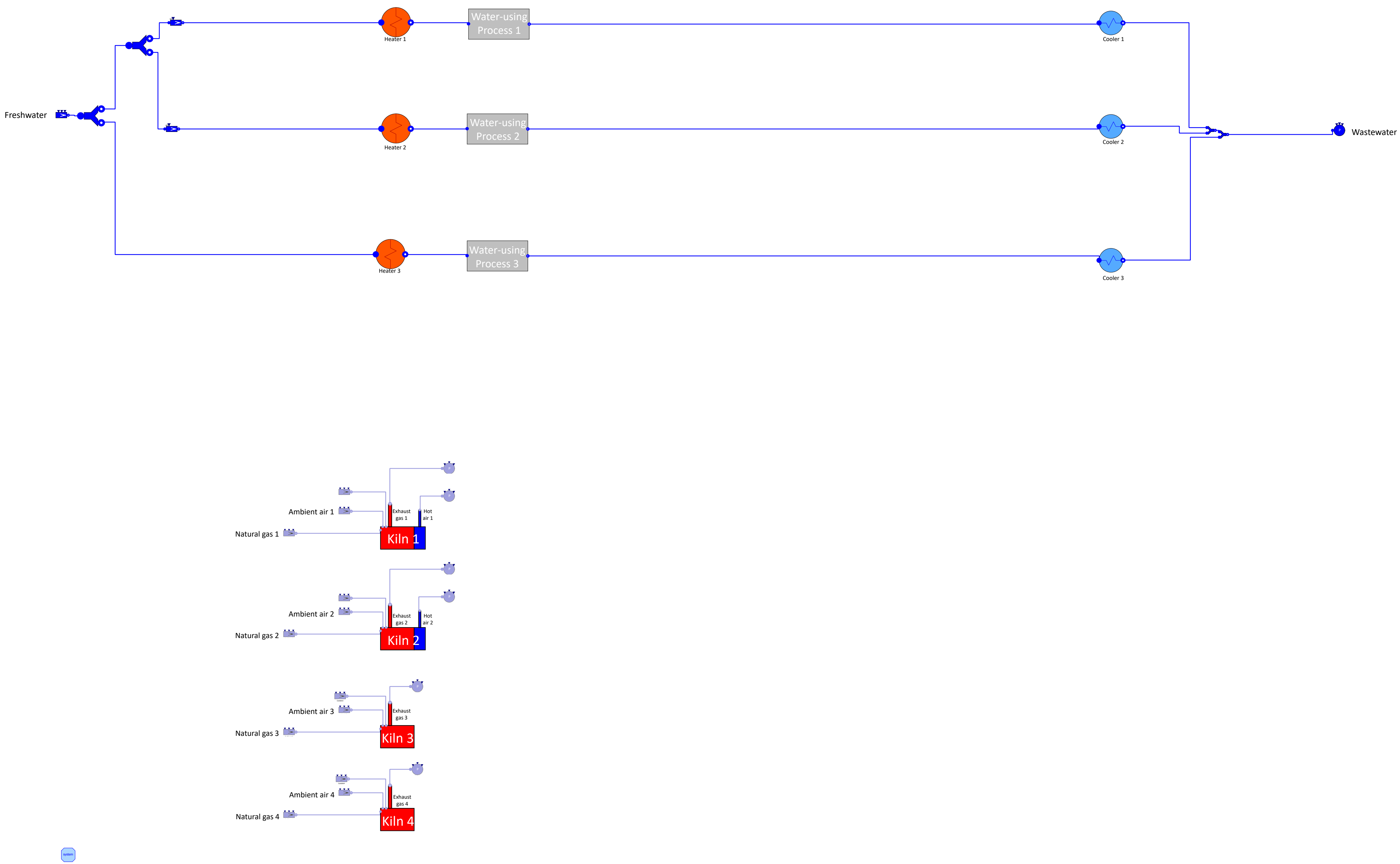


Figure 4.12. Flowsheet assembling of Baseline Scenario using the ThermWatt Modelica library capabilities

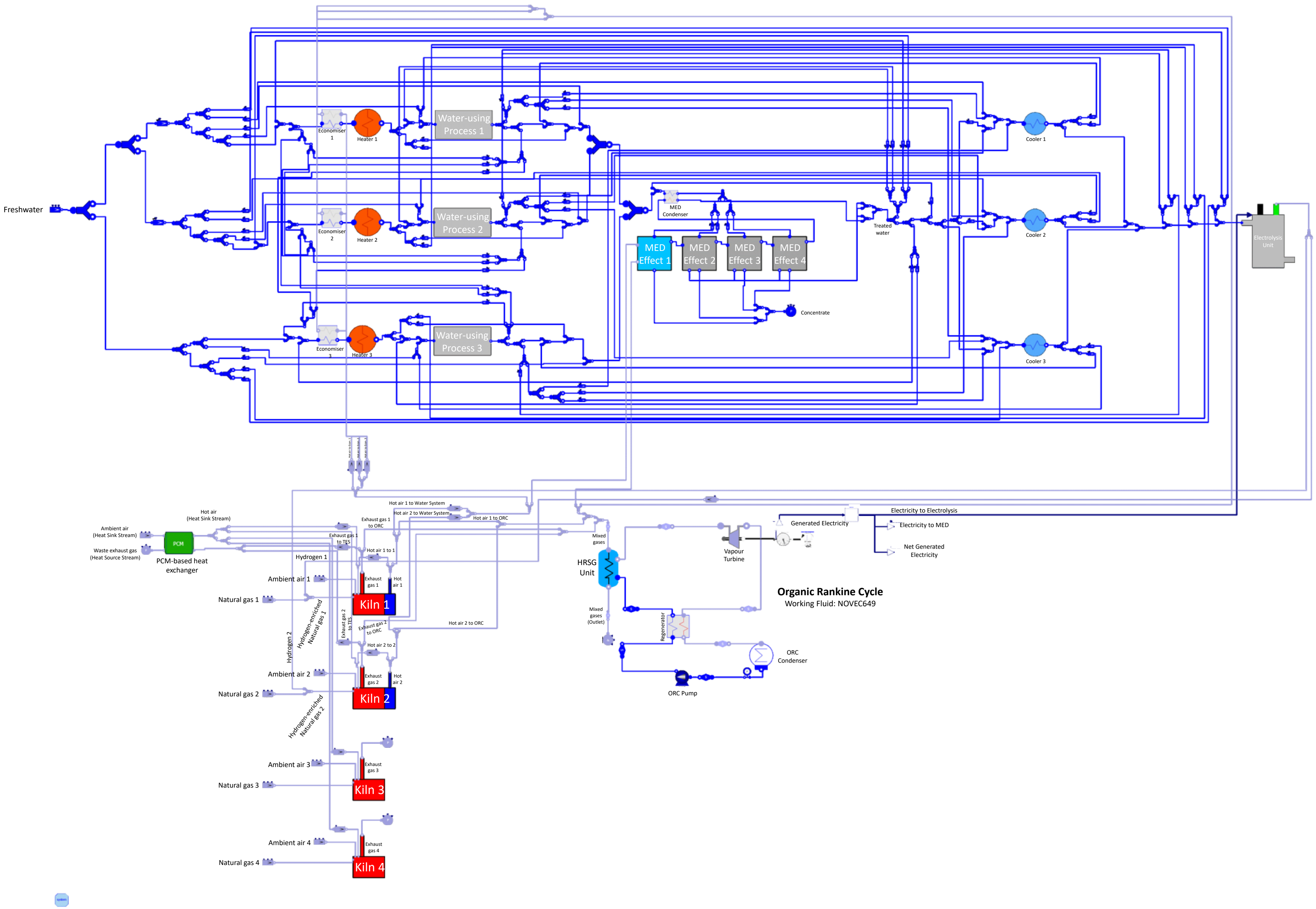


Figure 4.13. Flowsheet assembling of Scenario 1 using the ThermWatt Modelica library capabilities

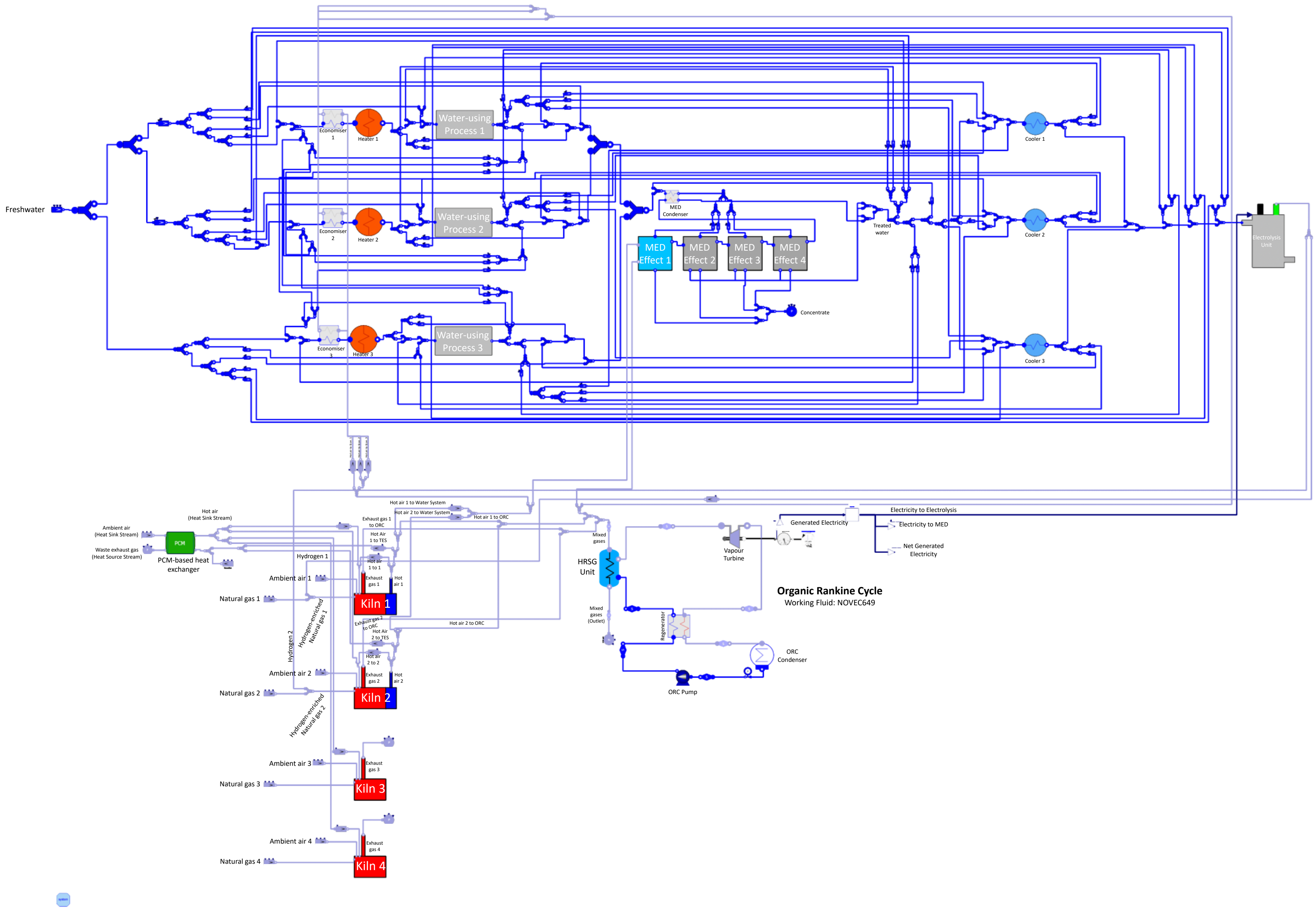


Figure 4.14. Flowsheet assembling of Scenario 2 using the ThermWatt Modelica library capabilities

Scenario Analysis

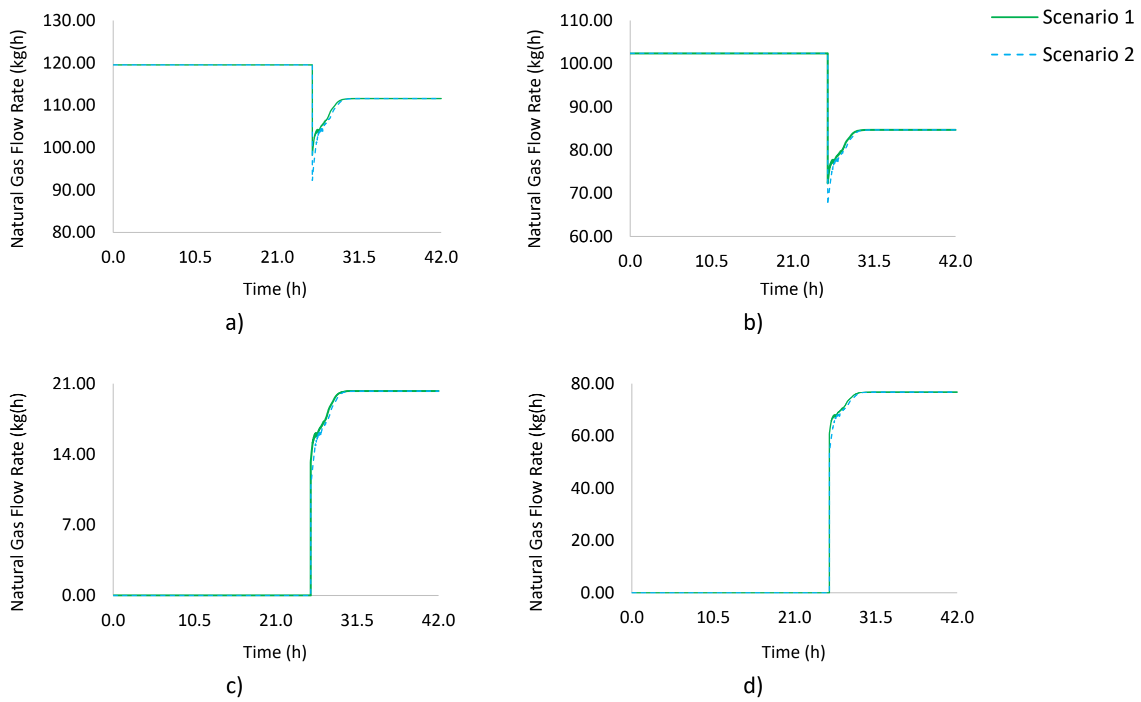
The conceptualized scenarios 1 and 2 are set to assess which one has the highest potential in terms of the reduction of the total cost over the total time of a charge/ discharge cycle. For the performance of the scenario analysis for the presented case-study, a set of parameters related to stream recirculation was considered common for both scenarios, so to establish a basis of comparison. The basis of comparison in this case was established by the maintenance of determinate parameters related to stream recirculation at common values for both scenarios, in addition to the maintenance of equivalent values for different sets of stream recirculation (for instance, the mass flow rate of the recirculated air stream to the TES unit in Scenario 1 is set as the same numerical value as the mass flow rate of the exhaust gas stream to the TES unit in Scenario 2). The following procedure was taken into account (subsisting on the definition of common values for key parameters of the system with the sole purpose of establishing a basis of comparison between scenarios):

- The mass flow rate of the recirculated hot air stream is set at 5000 kg/h for both Kiln 1 and 2 in both Scenario 1 and 2;
- The mass flow rate of the recirculated hot air stream and the exhaust gas steam to the TES unit in Scenario 1 and 2 respectively was set as 5000 kg/h for both Kiln 1 and 2;
- The mass flow rate of the recirculated hot air stream to the water system was set as 5000 kg/h for both Kiln 1 and 2 in both Scenario 1 and 2;
- From the total hot air recirculated to the water stream, a quantity of 1000 kg/h was recirculated to each one of the three economisers installed in the water system in both Scenario 1 and 2;
- The mass flow rate of the hot air streams recirculated to the economisers were set so to allow the hot utility consumption on the heaters of the water system to be null in both Scenario 1 and 2;
- The mass flow rate of the treated water stream not recirculated from the outlet of the MED unit was set as null, to allow for the cold utility consumption in the water system coolers to be null as well in both Scenario 1 and 2;
- For the hydrogen production cases, a quantity of 62.34 kg/h of the outlet water stream from the water system is considered. Such corresponds to the quantity of water stream that would be recirculated to the inlet of water-using process 3, and in this case it is instead directed to the Electrolysis unit.

The comparison between the two conceptualized scenarios in this case-study is proceeded through the comparison of the total operational costs corresponding to a full charge/ discharge cycle (in €/cycle units), rather than in hourly-based costs (in €/h units). Such procedure is adopted to ensure that the TES unit is charged with the maximum possible thermal energy and it discharges the whole quantity of this stored energy to the heat sink stream (in this case, the inlet air stream). The operational costs are calculated as the sum of all water and energy use-related cost parcels, in a similar manner to the procedure taken for case-study 1. In Table 4-8, the results for energy and water use indicators obtained for each one of the elaborated scenarios for case-study 2 is presented. In Figures 4.15 and 4.16, simulation results for the mass flow rate of natural gas at the inlet of each kiln and the generated electricity along the operational time are presented. For the convenience of the explanation of results, in Figure 4.17 the time-dependant profile relative to the mean temperature of the PCM within the PCM-based heat exchanger are also presented.

Table 4-8. Results for the scenario analysis of Case-study 2

Utility/ Cost Parcel		Baseline	Scenario 1		Scenario 2	
			With Electricity Production	**With Hydrogen Production**	**With Electricity Production**	**With Hydrogen Production**
Thermal Process System						
Natural Gas Flow Rate (kg/cycle)	**Kiln 1**	5355.00	4872.45	4872.45	4867.24	4867.24
	Kiln 2	5044.20	3992.10	3931.88	3987.35	3927.14
	Kiln 3	334.29	324.27	324.27	321.60	321.60
	Kiln 4	1266.05	1245.40	1245.40	1239.12	1239.12
Net Generated Electricity (kWh/cycle)			1437.81		1437.55	
Total Operational Cost (k€/cycle)		12.80	10.92	11.07	10.90	11.05
Water System						
Freshwater Flow Rate (kg/h)		859.69	418.43	459.69	418.43	459.69
Total Operational Cost (€/h)		19.10	0.77	0.85	0.77	0.85
Overall						
Total Operational Cost (M€/year)		2.53	2.04	2.07	2.04	2.07



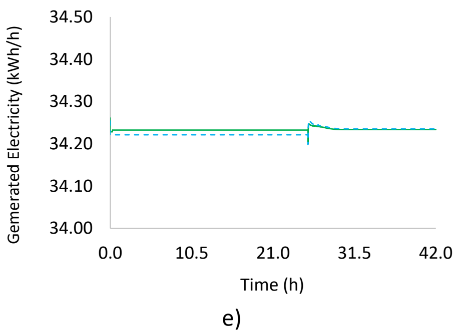


Figure 4.15. Simulation results for the mass flow rate of the natural gas at the inlet of a) Kiln 1, b) Kiln 2, c) Kiln 3 and d) Kiln 4, as well as e) Generated electricity (for the cases considering Electricity Production)

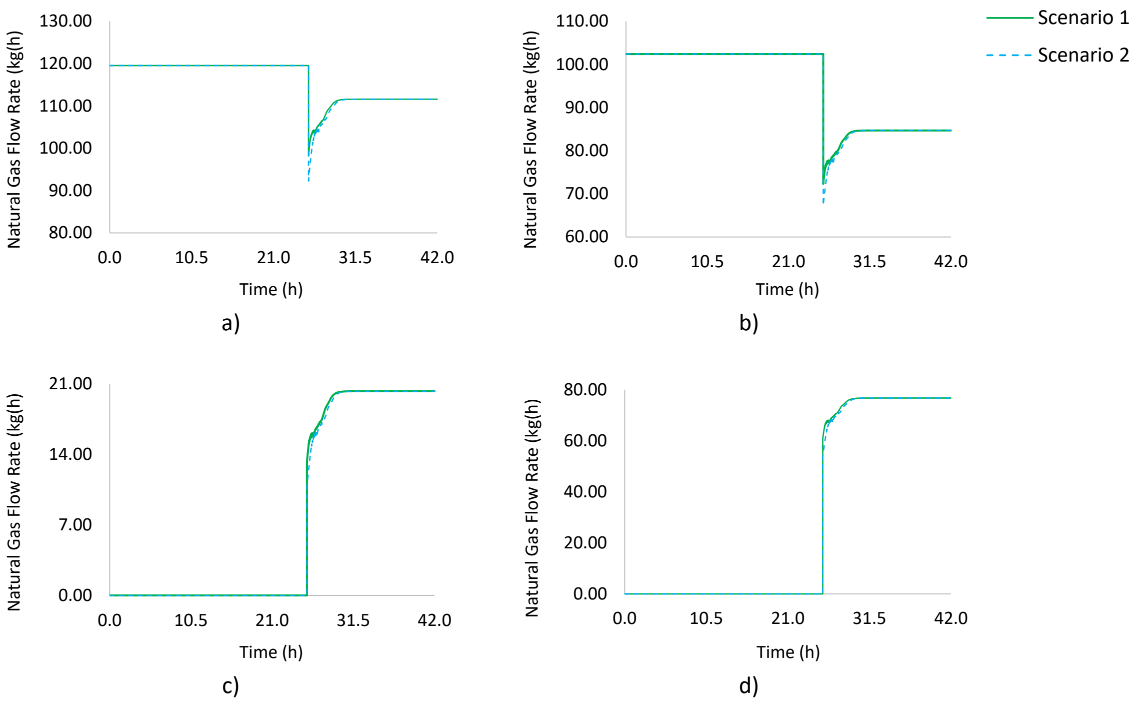
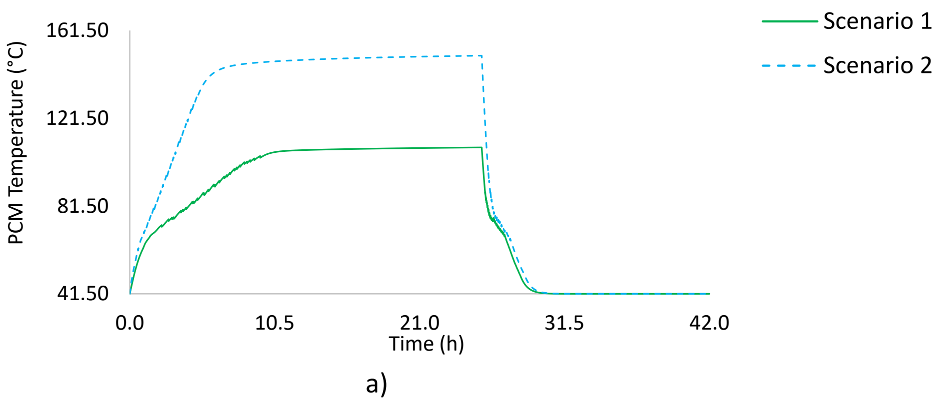
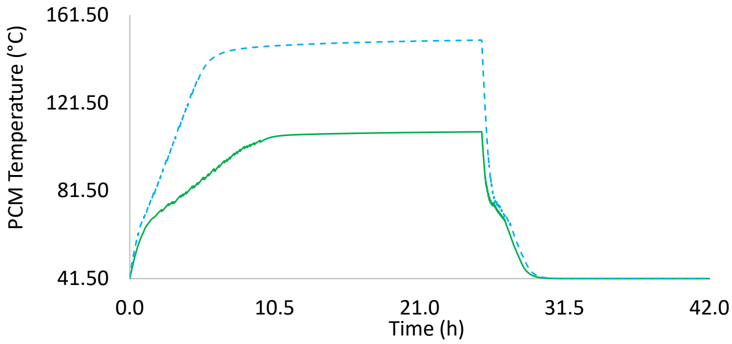


Figure 4.16. Simulation results for the mass flow rate of the natural gas at the inlet of a) Kiln 1, b) Kiln 2, c) Kiln 3 and d) Kiln 4 (for the cases considering Hydrogen Production)





b)

Figure 4.17. Simulation results for the temperature of the storage material within the PCM-based heat exchanger for the case of a) Electricity Production, b) Hydrogen Production

The total operational cost indicators considered in Table 4-8 were calculated by the summation of the costs associated to each energy parcel and freshwater, based on unitary values (baseline year of 2022) for the Portuguese industrial sector associated to each one of the considered parcels:

- 23.66 €/GJ for natural gas [378];
- 0.1459 €/kWh for electricity [379];
- 1.8499 €/m^3 for freshwater [380].

As may be verified by the analysis of Table 4-8 and Figures 4.15 – 4.17, Scenario 2 is the one with the highest cost reduction and therefore eco-efficiency promotion potential. The following verifications support such affirmation:

- The recirculation of hot air in favour of exhaust gas is associated to a superior capacity of storage of enthalpy within the PCM-TES unit for the same amount of charge time, as may be verified by the lower levels of mass flow rate of the natural gas streams at the inlet of each kiln obtained for Scenario 2;
- Such verification is supported by the results presented in Figure 4.17, in which the PCM temperature to which the thermal equilibrium is verified is higher for hot air recirculation (Scenario 2), which is attributed to a higher enthalpy having been store within the PCM-TES unit;
- The convergence to a higher PCM temperature (and thus a superior quantity of stored enthalpy) is attributed to a higher temperature of the heat source stream in Scenario 2 for the same recirculated mass flow rate;
- The availability of a higher quantity of hot air to be recirculated to the HRSG unit of the ORC system is able to generate a considerably higher quantity of electricity, although not the sufficient quantity for the compensation in terms of the savings on total operational costs;
- For both Scenarios 1 and 2, the case of the use of generated electricity as a direct use for electric energy savings in the plant instead of its use on the Electrolysis unit for hydrogen production compensates in terms of total operation costs savings.

5. Process and Energy System Optimisation

The newly developed simulation models presented in chapter 4 are prepared to map all the potential recirculation of water and energy streams on the process of conceptualizing the Water and Energy Integration Systems (WEIS) (as well as to assess several scenarios based on different inputs for key parameters), but not to assess the optimal point in which a determinate objective is attained (a numerical objective related to the optimal eco-efficiency point is set to be achieved for each case-study). In this chapter, optimisation models for each one of the approached case-studies are developed with the aim to assess the optimal operational points (in this case, the respective points in which total operational costs are minimum, indirectly provoking the maximization of eco-efficiency). For each case-study the optimisation model setup (in terms of decision variables, constraints and objective-functions) is defined and the optimisation results are presented. Further sensitivity analyses are performed based on the still existing uncertainty related to the obtainment of optimal results. In the end, a post-processing procedure based on an economic and environmental impact assessment is proceeded (being based on the calculation of the payback time and the absolute equivalent carbon dioxide emissions reduction indicators). A set of simplifications are performed in terms of fluid properties determination, namely in terms of the temperature – specific enthalpy correlations which are characterized in Table A3 of appendix A4.

A set of scientific publications by the authors extensively detail the development aspects associated to the presented models in terms of optimisation methodology adaptation and the aspects related to the development of an optimisation model for a WEIS [347,381].

5.1. Optimisation Models for Case-study 1

In this section, the development of the optimisation model for case-study 1 and the results obtained by the running of this model are presented. The development of this model takes into account the scenario defined as the most favourable in section 4.1. This optimisation model was developed using the GEKKO Python package [382]. The Python 3.11 version software was used for the running of the model. The internal IPOPT software and MUMPS solver of GEKKO package were used for the running of the model.

Formulation of the Optimisation Problem

The solving of the optimisation problem in question is set to be based on the use of the non-linear programming (NLP) methodology. Such methodology is selected due to requirement of the definitions of the mass balance, enthalpy balance and heat transfer that define the system, which are formulated as equality constraints. The objective-functions, in its turn, depend essentially on the energy and water utilities inputs on a system, thus being constituted by linear terms only. In this section, the characterization of the optimisation problem is presented in an aggregated manner, with the decision variables and constraints being presented in respective categories.

Since the present optimisation model has been developed on the basis of the simulation model presented in section 4.1, it is characterized by the same exact set of equations and variables that characterize the simulation model (the variables characterizing the simulation model are the decision variables of the optimisation models and the governing equations of the simulation model are formulated as equality constraints of the optimisation model). The full characterization of the optimisation problem in terms of all the defined decision variables and constraints is presented in appendix A5 (in which the Python code for the developed optimisation model is presented).

i) Decision Variables

The decision variables required for the definition of the optimisation problem consist in all the variables that characterize the Water and Energy Integration System (WEIS). It is to note that determinate system parameters do not vary for the required analysis, as these are not affected by changes of the values of the remaining variables that defined the mass and enthalpy balances of the system. In Table 5-1, the decision variables and relevant inequality constraints set for the described optimisation model are characterized.

Table 5-1. Characterization of decision variables and relevant inequality constraints for case-study 1

Decision Variables			
Category	**Variable**		
Thermal Process System			
Stream-related	• Natural gas flow rates ($\dot{M}_{Fuel}$) • Ambient air flow rates ($\dot{M}_{Amb.Air}$) • Exhaust gases flow rates ($\dot{M}_{Ex.}$) • Exhaust gases specific enthalpies ($h_{Ex.}$) and temperatures ($T_{Ex.}$))	• Hot air flow rates ($\dot{M}_{Hot\ Air}$) • Hot air specific enthalpies ($h_{Hot\ Air}$)/ temperatures ($T_{Hot\ Air}$) • Recirculated air flow rates ($\dot{M}_{Rec.Air}$) • Recirculated air specific enthalpies ($h_{Rec\ Air}$)/ temperatures ($T_{Rec\ Air}$)	
Sizing-related	• Generated electricity ($Elec$) • Electricity to MED unit ($Elec_{MED}$) • Electricity to Electrolysis unit ($Elec_{Electr.}$) • Net generated electricity ($Elec_{Eff}$)		
Water System			
Stream-related	• Freshwater mass flow rate ($\dot{M}_{FW}$) • Each water stream mass flow rate ($\dot{M}_{w}$) • Each water stream specific enthalpy (h_{W})/ temperatures (T_{W}) • Each water stream contaminant concentration (C_{W})		
Sizing-related	• Heat transfer area of economisers ($A_{Econ.}$) • Heat transfer area of MED Effect 1 (A_{Eff1})		
Relevant Inequality Constraints			
Variable		**Lower Bound**	**Upper Bound**

Thermal Process System		
Temperature of Mixed Gas at the outlet of the ORC ($T_{ORC,Out}$) (ºC)	75	
Water System		
Salt concentration of the inlet water stream in each water-using process ($C_{w,WP,in}$)	200.00	
Salt concentration of the inlet water stream in each water-using process ($C_{w,WP,out}$)	800.00	1000.00
Salt concentration of the remaining water streams in the water system ($C_{w,WS}$)	0.00	1000.00

It is to note that the corresponding pairs of temperature and specific enthalpy are mentioned within the same category since these variables are considered correspondents in terms of equation enunciation (temperature variables are used for heat transfer equations and specific enthalpies for enthalpy balances due to less exhaustive requirements of enunciation of equality constraints). The considered correspondence between temperature and specific enthalpy for different media is established in appendix A4. The same procedure for the temperature/ specific enthalpy correspondence was taken for further models.

ii) Constraints

The constraints set to be defined for the proposed optimisation correspond to limit values (minimum and/ or maximum) necessary to be considered for several variables (inequality constraints) and the mass balance, enthalpy balance and heat transfer equations that characterize the conceptualized WEIS superstructure (equality constraints). In the formulation of the optimisation problem, it was taken a procedure in which all the parameters that characterize the system having appreciable variations were defined as decision variables, with the maximum possible number of decision variables being considered in the definition of the problem. Such procedure disables the necessity to define any inequality constraint by mathematical formulation (these consists only in the limit values of decision variables). In Table 5-2, the equality constraints set for the described optimisation model are characterized.

Table 5-2. Definition of equality constraints for case-study 1

Thermal Process System	
$\dot{M}_{Fuel,Baseline} \cdot LHV_{NG} = \dot{M}_{Fuel} \cdot LHV_{Fuel} + \dot{M}_{Comb.Air} \cdot (h_{C.Air} - h_{C.Air,Baseline})$	(5.1)
$\dot{M}_{C.Air} = \dot{M}_{Rec.Air} + \dot{M}_{Amb.Air}$	(5.2)
$\dot{M}_{C.Air} \cdot h_{C.Air} = \dot{M}_{Rec.Air} \cdot h_{Rec.Air} + \dot{M}_{Amb.Air} \cdot h_{Amb.Air}$	(5.3)
$\dot{M}_{Fuel} + \dot{M}_{Comb.Air} = \dot{M}_{Ex.}$	(5.4)
$\dot{M}_{Fuel} \cdot AF = \dot{M}_{Comb.Air}$	(5.5)
$AF \cdot LHV_{NG} = AF_{Baseline} \cdot LHV_{Fuel}$	(5.6)
$LHV_{Fuel} = Y_{NG} \cdot LHV_{Natural\,Gas} + Y_{H_2} \cdot LHV_{H_2}$	(5.7)
$\dot{M}_{gas,in,ORC} \cdot (h_{gas,in,ORC} - h_{gas,out,ORC}) \cdot 0.0571 = Elec$	(5.8)
$Elec = Elec_{MED} + Elec_{Electr.} + Elec_{Eff}$	(5.9)
Water System	
$\dot{M}_{W.,to-be-splitted} = \sum_{i=1} \dot{M}_{W.,split,i}$	(5.10)
$h_{W.,to-be-splitted} = h_{W.,split,i}$	(5.11)

$C_{W.,to-be-splitted} = C_{W.,split,i}$	(5.12)
$\sum_{i=1} \dot{M}_{W.,to-be-mixed,i} = \dot{M}_{W.,mixed}$	(5.13)
$\sum_{i=1} (\dot{M} \cdot h)_{W.,to-be-mixed,i} = (\dot{M} \cdot h)_{W.,mixed}$	(5.14)
$\sum_{i=1} (\dot{M} \cdot C)_{W.,to-be-mixed,i} = (\dot{M} \cdot C)_{W.,mixed}$	(5.15)
$\dot{M}_{W.,in,Eff} \cdot {}^{1}/_{5} = \dot{M}_{TW.,Eff} + \dot{M}_{Concentrate,Eff}$	(5.16)
$q_{with.,MED} - \dot{M}_{TW.,Eff1} \cdot (h_{V,Eff1} - 418.90) = \dot{M}_{W.,in,Eff1} \cdot {}^{1}/_{5} \cdot (418.90 - h_{w,in,Eff})$	(5.17)
$\dot{M}_{TW.,Eff\,k-1} \cdot (h_{V,Eff1} - 418.90) = \dot{M}_{TW.,Effk} \cdot (h_{V,Effk} - 418.90) + \dot{M}_{W.,in,Effk} \cdot {}^{1}/_{5} \cdot (418.90 - h_{w,in,Eff})$	(5.18)
$\dot{M}_{TW.,Effect} \cdot (2675.43 - 418.90) = \dot{M}_{W.,in,Eff} \cdot {}^{1}/_{5} \cdot (h_{Vapour,Eff1} - 418.90)$	(5.19)
$q_{with.} = U \cdot A \cdot \left((T_{Air,in} - T_{w,out}) \cdot (T_{Air,out} - T_{w,in}) \cdot \left((T_{Air,in} - T_{w,out}) + (T_{Air,out} - T_{w,in})\right) \cdot 0.5\right)^{1/3}$	(5.20)
$Elec_{MED} = 2.5 \cdot {}^{\dot{M}_{TW}}/_{999}$	(5.21)
${}^{\dot{M}_{DW,Eff}}/_{0.0180} \cdot X_{H_2} = {}^{\dot{M}_{H_2}}/_{0.0020}$	(5.22)
${}^{\dot{M}_{DW,Eff}}/_{0.0180} \cdot 285.85 \cdot X_{H_2} = 0.70 \cdot Elec_{Electrolysis} \cdot 3600$	(5.23)

In relation to the constant values presented throughout Table 5-2, is to note:

- 0.0571 refers to the thermal-to-electric conversion efficiency associated to the Organic Rankine cycle (ORC);
- ${}^{1}/_{5}$ refers to the splitting of the water stream at the outlet of the Multi-effect distillation (MED) unit condenser to each one of the five effects;
- 418.896 (with kJ/kg units) refers to the specific enthalpy of saturated liquid water;
- 2675.43 (with kJ/kg units) refers to the specific enthalpy of saturated steam;
- 2.5 (with kWh/m^3 units) refers to the specific electricity consumption of the MED unit (per volumetric unit of produced treated water);
- 999 (with kg/ m^3 units) refers to the density of liquid water;
- 0.0180 (with kg/mol units) refers to the molar mass of water;
- 0.0020 (with kg/mol units) refers to the molar mass of molecular hydrogen;
- 285.85 (with kJ/mol units) refers to the specific enthalpy of the reaction of water splitting;
- 0.70 refers to the electric-to-reaction enthalpy efficiency associated to the Electrolysis unit;
- 3600 (with kJ/kWh units) refers to the factor of conversion of kWh to kJ energy units.

Considering the presented decision variables and equality constraints, the present optimisation model contains 66 degrees of freedom.

iii) Objective-Function

The objective-function for the proposed optimisation problem shall reflect the real-life operational aim corresponding to the minimisation of energy (either natural gas in combustion-based processes, hot utilities or cold utilities) and water use in the case-study ceramic plant. Such formulation passes by the conversion of energy and water consumption levels in a hourly basis (kg/h for natural gas, GJ/h for hot and cold utilities and m^3/h for freshwater) to hourly-based monetary values (in €/h). For this end, the following procedure was taken based on reference unitary prices for the industrial sector:

- The unitary value of 23.66 €/GJ was considered for natural gas [378];
- The unitary value of 0.1459 €/kWh was considered for electricity [379];
- The unitary price of 1.8499 €/ m^3 was considered for freshwater [380].

The formulated objective-function is presented in equation (5.24).

$$\min\Big(23.66(€/\mathrm{GJ})\cdot 0.0453(\mathrm{GJ/kg})\cdot \dot{\mathrm{M}}_{\mathrm{NG}}(\mathrm{kg}) + 1.8499(€/\mathrm{m^3})\cdot {}^{1}/_{999}\,(\mathrm{m^3/kg})\cdot \dot{\mathrm{M}}_{\mathrm{FW}}(\mathrm{kg/h}) + 23.66(€/\mathrm{GJ})\cdot \mathrm{q}_{\mathrm{Hot.Ut.}}(\mathrm{GJ/h}) + 0.1459(€/\mathrm{kWh})\cdot\frac{1}{0.95}\cdot\frac{1}{3600}(\mathrm{kWh/GJ})\cdot \mathrm{q}_{\mathrm{Cold.Ut.}}(\mathrm{GJ/h}) + 0.1459(€/\mathrm{kWh})\cdot \mathrm{Elec}_{\mathrm{Eff}}(\mathrm{kWh/h})\Big)(€/\mathrm{h}) \tag{5.24}$$

Optimisation Results

The running of the optimisation model allows the obtainment of results associated to each one of the streams the characterize the conceptualized WEIS. As the optimisation problem has as a basis the superstructure for this case-study presented in section 4.1, the running of this model allows to obtain values for each mass flow rate associated to each stream, even null for determinate streams (meaning these streams ultimately do not exist in the optimised configuration). The running of the model is also set for the obtainment of values associated to the use of each one of the energy and water-related utilities (natural gas in tunnel kilns, freshwater, hot and cold utilities of the water system and generated electricity). In Table 5-3, the results obtained for the optimised use of each one of the energy and water use-related inputs is presented alongside the corresponding baseline values (the initial case in which any improvement measure has still been implemented) and the values obtained for the scenario analyses presented on section 4.1.

Table 5-3. Optimisation results for the main energy and water use indicators

Utility/ Cost Parcel		Baseline	Scenario 1		Optimised
			With Electricity Production	With Hydrogen Production	
Thermal Process System					
Natural Gas Flow Rate (kg/h)	**Tunnel Kiln 1**	196.5	160.38	156.56	160.48
	Tunnel Kiln 2	103.5	90.21	90.21	74.27
Net Generated Electricity (kWh/h)			91.66		84.22
Water System					
Freshwater Flow Rate (m^3/h)		1.378	0.937	0.996	1.298
Hot Utility Consumption (GJ/h)	**Heater 1**	0.175			
	Heater 2	0.183			
	Heater 3	0.133			
	Heater 4	0.023			
Cold Utility Consumption (GJ/h)	**Cooler**	0.396		0.018	0.002

		Overall		
Total Operational Cost (€/h)	350.88	255.75	265.16	240.69
Total Operational Cost (M€/year)	2.745	2.001	2.080	1.883

As may be observed in Table 5-3, the solving of the optimisation problem converges to a point in which the total operational costs (the summation of each one of the energy and water-related cost parcels) are significantly lower than the corresponding baseline value and the values obtained for the previously elaborated scenario analyses. As such, it may be considered that the solving of the optimisation problem has been primarily successful in respect to the achievement of the proposed objective of assessing potential energy and water use-related improvements.

In respect to the comparison between the results obtained for the scenario analyses and the ones obtained by optimisation, the following verifications may be pointed out:

- The reduction of total operational costs associated to the optimised configuration is essentially attributed to the reduction of natural gas consumption on the two tunnel kilns, especially on tunnel kiln 2 (although a comparable reduction level is verified for tunnel kiln 1, the natural gas flow rate for the optimised scenario is slightly higher than the simulated scenario considering Electricity Production, with the highest difference between simulated and optimised values being attributed to tunnel kiln 2);
- The quantity of generated electricity in the optimised scenario is slightly lower compared to the simulated scenario with Electricity Production, although being maintained a comparable electricity generation level so to be possible for the total operational costs to be lower;
- The solving of the optimisation problem converges to a point in which the hot utility consumptions within the water system is zero (similar to the configuration adopted for the simulated scenarios), as well as a negligible quantity of cold utility consumption;
- Attending to the significantly lower unitary price associated to freshwater consumption in comparison to the energy-related prices (1.8499 €/ m^3, corresponding to $1.852 \cdot 10^{-3}$ €/kg, for freshwater, compared to 23.66 €/GJ, corresponding to 1.067 €/kg, for natural gas and 0.1459 €/kWh for electricity), it is possible to verify that the solving of the optimisation problem converges to a point in which the reduction of freshwater flow rate is significantly high.

In Figure 5.1, the results obtained for the parameters of each stream of the WEIS and sizing variables (heat transfer areas) are presented.

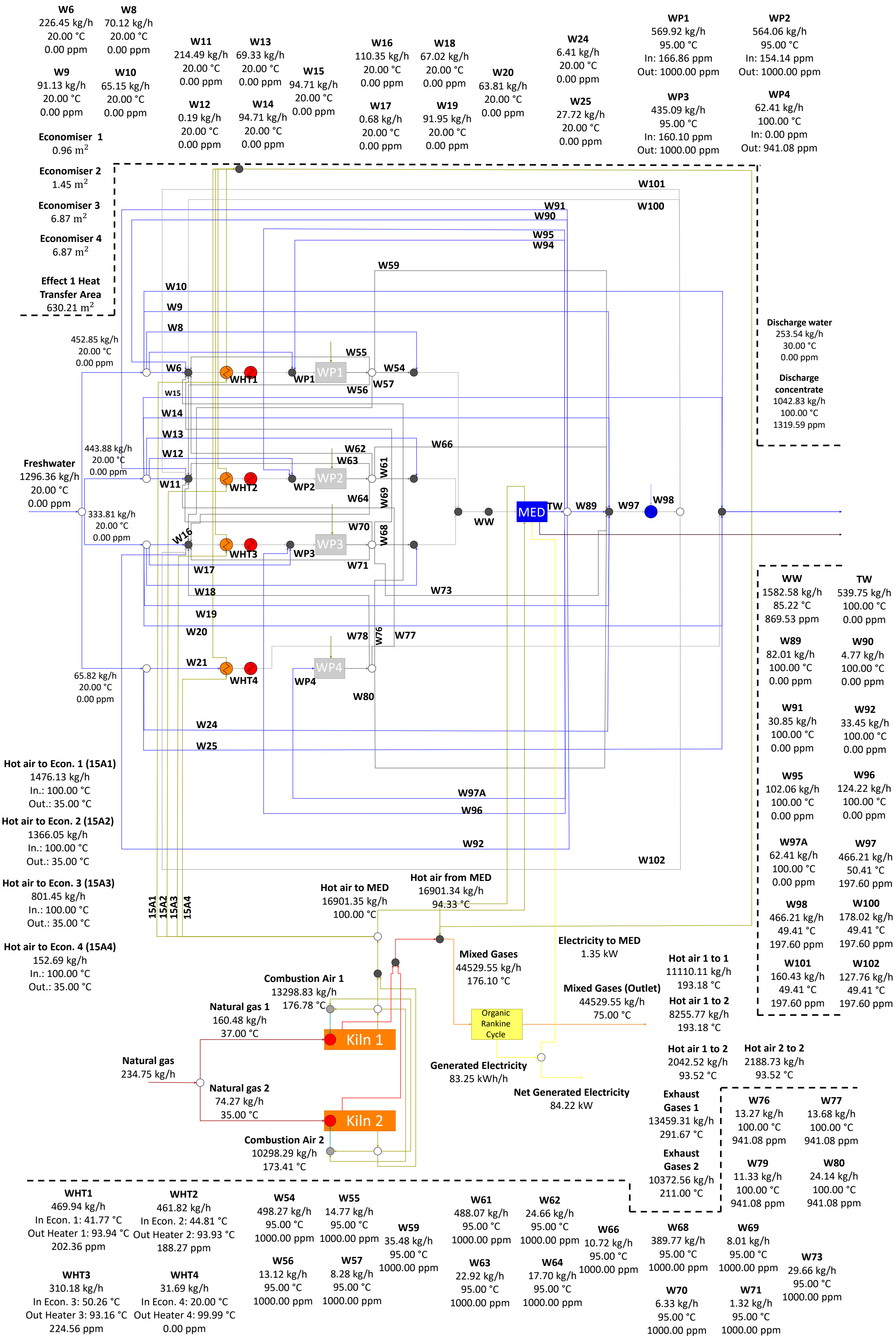


Figure 5.1. Flowsheet of the optimised WEIS configuration for case-study 1

Sensitivity Analysis

The optimisation model developed for the purpose of the obtainment of the results presented in the previous section is set to be submitted to a sensitivity analysis with the aim to assess the impact of the alteration of key parameters that characterize the model on the obtained results. Such procedure is taken to test the robustness of the developed model to punctual alterations on determinate parameters values, so to verify potential assumptions taken for the definition of such values by not altering the whole model in terms of formulation. The parameters whose values are set to be varied are minimum and maximum values associated to decision variables, as these are the ones whose definition assumptions are set to be analysed. Other values set as constant are fixed values whose variation would be considered as an alteration of the model in terms of formulation (with the exception of the thermal-to-electric conversion efficiency associated to the ORC, which is an operational parameter associated to a certain uncertainty which must be analysed).

The present sensitivity analysis was performed by adopting a one-at-a-time (OAT) procedure, in which the value associated to a single parameter category is varied. The handling of this procedure was based on the variation of two categories of parameters:

- The upper bound of the salt concentration associated to water streams (excluding the inlet and outlet streams to and from the water-using processes);
- The thermal-to-electric energy conversion associated to the ORC.

In the context of the effectiveness of the final optimisation results, the present sensitivity results are set to generate an adjustment scenario that is set to potentially supplant the initial optimisation results (by analysing a set of scenarios generated by the input of several different values for the aforementioned parameters). Such supplantation is set occur in the case that a balance between water and energy-use related benefits and optimisation modelling improvement are verified. The described sensitivity analysis is presented in Table 5-4.

Table 5-4. Sensitivity analysis results for Case-study 1

Variables	Adjustment	Natural gas consumption in tunnel kilns (kg/h)	Net generated electricity (kW)	Freshwater flow rate (m^3/h)	Hot utility consumption (MJ/h)	Cold utility consumption (MJ/h)	Discharge water flow rate (m^3/h)	Total operational costs (€/h)
Salt Concentration (ppm) / ORC efficiency				**1000.00**				
6.40%	**1**	234.75	84.22	1.298		1.98	0.254	240.69
6.00%	**2**	235.80	80.25	1.179		0.04	0.101	242.08
8.00%	**3**	240.11	110.89	1.027		13.96	0.126	242.53
Salt Concentration (ppm) / ORC efficiency				**2000.00**				
6.40%	**4**	237.19	86.36	1.295			0.275	242.89
6.00%	**5**	235.33	80.04	1.051			0.000	241.38
8.00%	**6**	235.61	107.09	1.067			0.000	237.76
Salt Concentration (ppm) / ORC efficiency				**900.00**				
6.40%	**7**	239.37	88.33	1.176	17.46	1.02	0.101	245.17
6.00%	**8**	236.01	80.22	0.984			0.031	241.95
8.00%	**9**	241.66	108.38	1.233		0.60	0.171	244.36

By the analysis of the sequence of Table 5-4, it is possible to perform the following primary verifications:

- The overall variations in terms the analysed indicators (which are in majority energy and water use-related indicators) are not significant, having been possible to obtain for all performed adjustments similar levels for natural gas consumption in each one of the tunnel kilns, hot utilities consumptions (which are null for most of the adjustments except one), cold utility consumption (it takes values lower than 2.00 MJ/h for all adjustments except one which are significant of a considerably low variation of temperature between the inlet and outlet water stream) and total operational costs;
- The most verifiable difference resides on the results obtained for freshwater consumption and discharge water flow rate. As such, it may be concluded that for the convergence of the optimisation problem in respect to the performed adjustments towards the obtainment of similar results for reduced energy use does necessarily provokes visible variations in terms of inlet freshwater quantity, which may be once again attributed to the lower unitary price for freshwater. In relation to the outlet discharge water, the flow rate levels may be interpreted at the light of a similar observation, since the higher level of freshwater input necessarily provokes a higher quantity of discharge water for the same level of water recirculation (counting that approximate levels of water recirculation within the water system are obtained for all the adjustments);
- The variations performed for the upper bound of the selected salt concentration-related variables are not necessarily linear with the variations of freshwater flow rate (as may be verified between the pair of adjustments 1/ 4, 4/ 7, 2/ 5, 2/ 8 and 5/ 8). In most corresponding pairs of adjustments (except the pair 1/ 4), these variations nonetheless provoke a considerable decrease on natural gas use in tunnel kilns and a reduction of total operational costs thereof. Such results may be potentially attributed to the promotion of recirculation of water within the water system owing to the relief on the salt concentration of certain streams. This recirculation in its turn cause also a promotion on the internal heat recovery within the water system, thus decreasing the dependence of hot air supply to the economisers. In its turn, this hot air is recirculated instead to the tunnel kilns to constitute a part of the pre-heated combustion air;
- The thermal-to-electric energy conversion efficiency associated to ORC was set as analysed parameter since this system is not directly modelled in the context of the optimisation model. As such, the corresponding adjustments represent points of the operation in which this thermal-to-electric energy conversion efficiency is respectively and considerably lower and higher than the one obtained by the simulation model. As may be verified, for most of the performed adjustments the relative increase of ORC thermal-to-electric conversion efficiency provokes a dislocation in relation to the obtained results to a point in which either freshwater flow rate or natural gas consumption in the kilns is lower, this is, the optimisation problem converges to a point in which electricity generation is favoured over natural gas and freshwater consumption reduction.

Attending to the aforementioned verifications, it may be concluded that although the initially developed optimisation model is robust in respect to result obtainment, minor improvements may be performed in terms of the relief of certain inequality constraints (namely the values considered for upper bounds). In the prospect to improve the initially obtained solution, the configuration obtained by adjustment 5 is then set as the one to be considered for further step of integration within the simulation model, as this is the one in which it is obtained a compromise between the highest possible reduction of total operational costs and the insurance of the obtainment of the most coherent results associated to electricity generation (in which the thermal-to-electric energy conversion efficiency is considerably decreased so to ensure that this parameter is certainly higher in the context of the running of the simulation model, thus ensuring that the definitive solution is the one associated to the minimum level of total operational costs).

In Table 5-5, the revised optimisation results and its comparison with corresponding previous results for the main water and energy use indicators are presented. The stream allocation configuration obtained associated to the adopted configuration following sensitivity analysis (corresponding to adjustment 5) is presented in Figure 5.2.

Table 5-5. Revised optimisation results for the main energy and water use indicators and its comparison with initial and previously obtained values

Utility/ Cost Parcel		Baseline	Scenario 1		Optimised (Revised)
			With Electricity Production	With Hydrogen Production	
Thermal Process System					
Natural Gas Flow Rate (kg/h)	Tunnel Kiln 1	196.5	160.38	156.56	156.53
	Tunnel Kiln 2	103.5	90.21	90.21	78.80
Net Generated Electricity (kWh/h)			91.66		80.04
Water System					
Freshwater Flow Rate (m^3/h)		1.378	0.937	0.996	1.051
Hot Utility Consumption (GJ/h)	Heater 1	0.175			
	Heater 2	0.183			
	Heater 3	0.133			
	Heater 4	0.023			
Cold Utility Consumption (GJ/h)	Cooler	0.396		0.018	
Overall					
Total Operational Cost (€/h)		350.88	255.75	265.16	241.38
Total Operational Cost (M€/year)		2.745	2.001	2.080	1.889

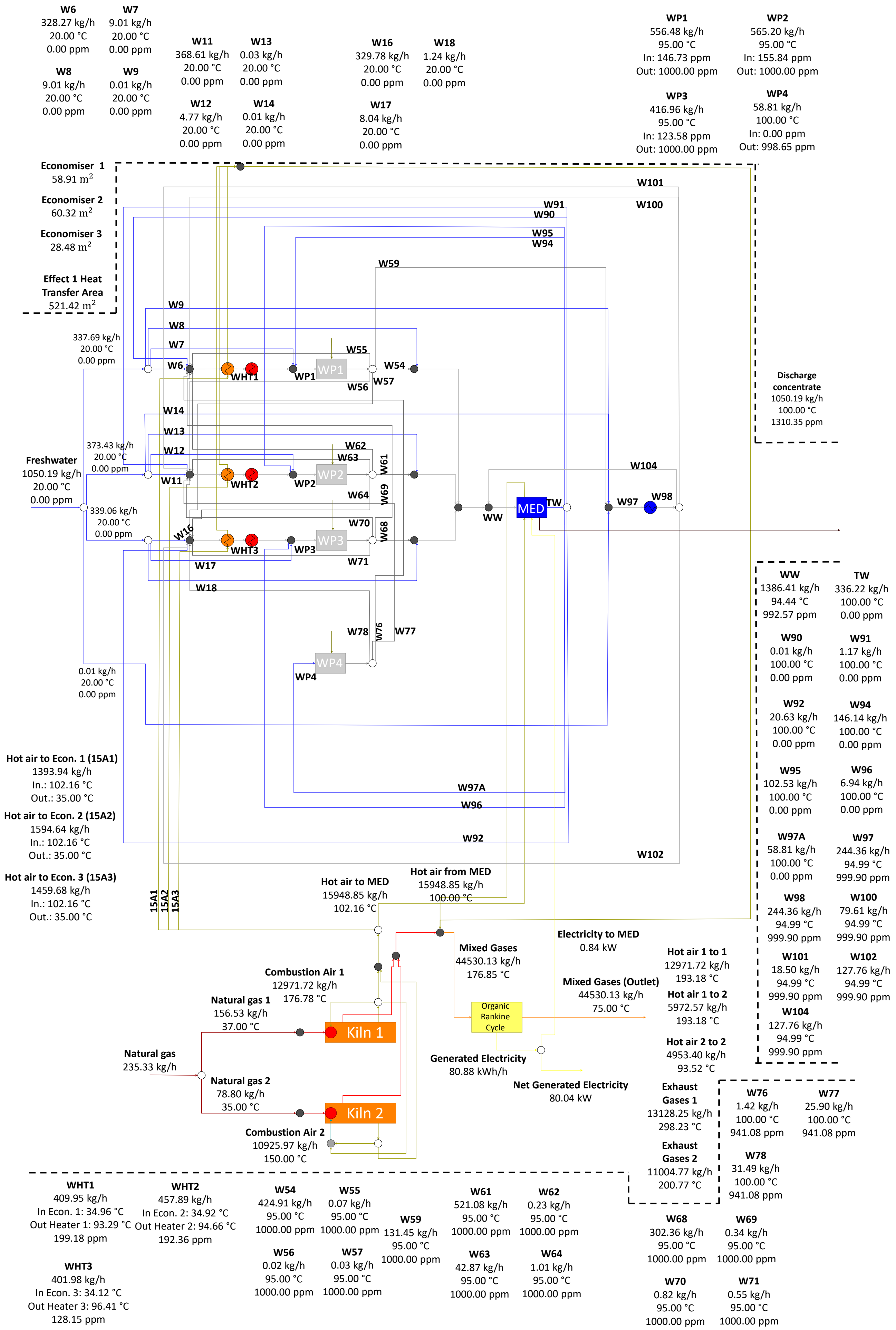


Figure 5.2. Flowsheet of the revised optimised WEIS configuration for case-study 1

Integration with the Simulation Model

The optimisation model presented in the previous section has been developed with the aim to determine the optimal operational conditions associated to the conceptualized WEIS, namely the values for stream allocation-associated and sizing parameters for which the energy and water use-related costs are the minimum possible. As mentioned afore, the model has been developed according to certain assumptions and simplifications. These may be summarized to the following:

- Assumptions associated to the inexistence of proper packages for the modelling of the properties of the involved fluids, which in this case led to the use of simplified formulas to determinate a set of properties (which is the case of specific enthalpies) and the assumptions of constant values for other (which is the case of densities);
- Simplifications related to the modelling of the ORC system within the optimisation model (which is summarized to the sole consideration of the parameter of thermal-to-electric energy conversion efficiency).

In Table 5-6, the comparison of the values associated to the main energy and water-use indicators obtained for all the phases of the exploitation of case-study (from the baseline case to the definitive optimisation configuration) are presented. In Figure 5.3, the flowsheet and stream allocation and sizing parameters values associated to the definitive optimised configuration are presented.

Table 5-6. Optimisation results for the main energy and water use indicators and its comparison with initial and previously obtained values

Utility/ Cost Parcel		Baseline	Scenario 1: With Electricity Production	Scenario 1: With Hydrogen Production	Optimised	Optimised (Definitive)
Thermal Process System						
Natural Gas Flow Rate (kg/h)	**Tunnel Kiln 1**	196.5	160.38	156.56	156.53	156.53
	Tunnel Kiln 2	103.5	90.21	90.21	78.80	78.80
Net Generated Electricity (kWh/h)			91.66		80.04	81.91
Water System						
Freshwater Flow Rate (m³/h)		1.378	0.937	0.996	1.051	1.051
Hot Utility Consumption (GJ/h)	**Heater 1**	0.175				0.004
	Heater 2	0.183				0.004
	Heater 3	0.133				0.003
	Heater 4	0.023				0.003
Cold Utility Consumption (GJ/h)	**Cooler**	0.396		0.018		
Overall						
Total Operational Cost (€/h)		350.88	255.75	265.16	241.38	241.35
Total Operational Cost (M€/year)		2.745	2.001	2.080	1.889	1.888

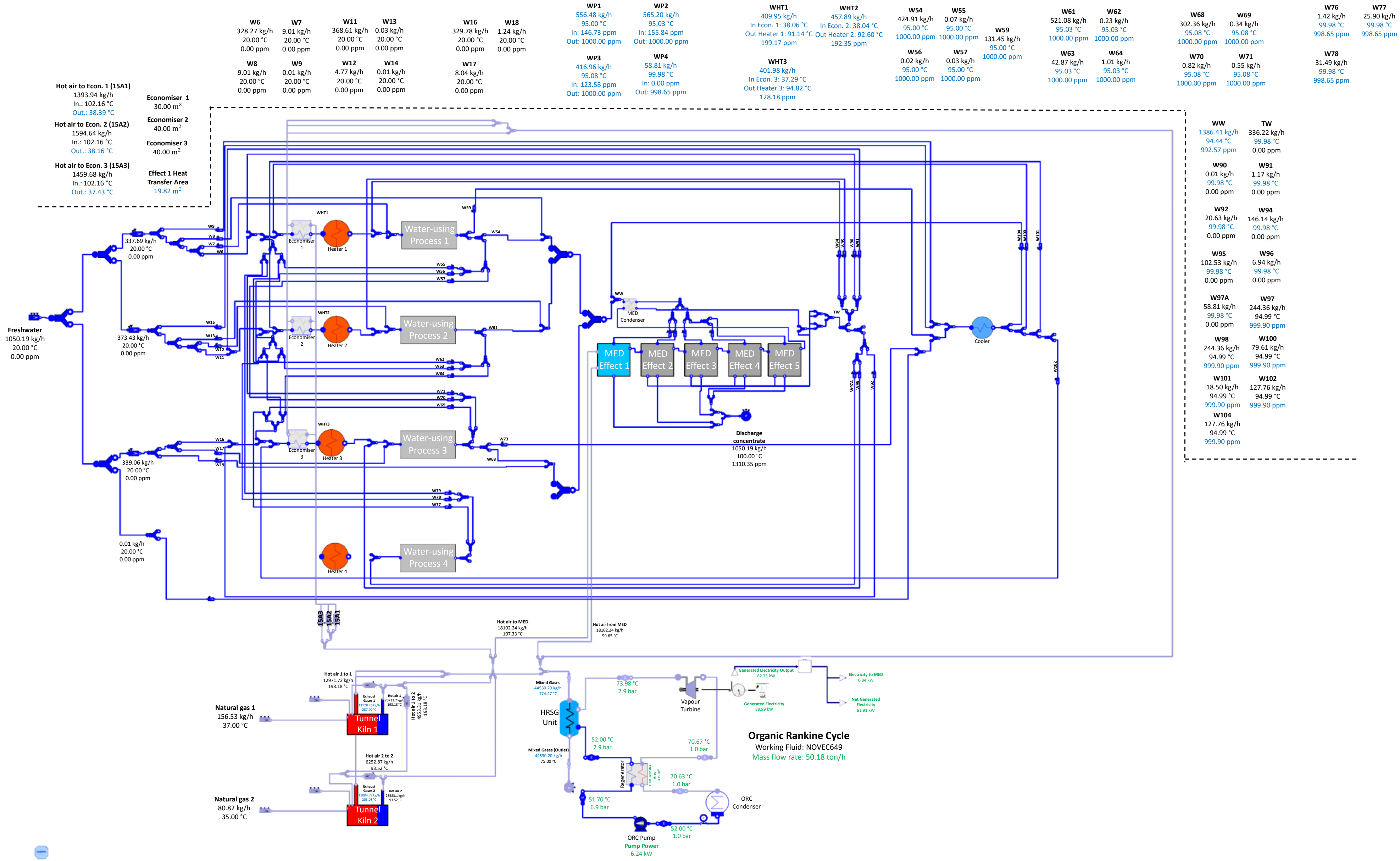


Figure 5.3. Flowsheet assembling of the Final Configuration using the ThermWatt Modelica library capabilities (darker colour: corresponding values to the optimisation model, lighter colour: referent to variables that are only part of the simulation model)

As mentioned afore, the obtainment of the definitive optimised values for the WEIS relies on the transference of the values obtained for the stream allocation and sizing-related parameters which have been obtained by the running of the optimisation model to the simulation model, by establishing a connection between the same variables for both model counterparts. In practice, such is performed using the OpenModelica Python package that has been integrated within the ThermWatt computational tool, in which the parameters values generated by the NLP model developed in Python are transferred to its Modelica counterpart. In this prospect, the Python model functions as necessary layer that is built over the Modelica model with the aim to obtain the most favourable values for the conceptualized installations in which the energy and water use is the minimum possible although by respecting all existing operational constraints. Such methodological arrangement generates a definitive model, in which it is simultaneously ensured the optimal solution for the conceptualized WEIS and the scientific accuracy of results.

The evaluation of the final model in terms of both validity and optimal results obtainment resides in the comparison of the results obtained between this model and the counterpart optimisation model developed with the Python GEKKO package. In relation to the aspect of the validity of the model, it may be verified by the comparative analysis of Figure 5.2 and 5.3 that the values obtained for the equivalent variables present a correspondence for most of the variables, being verified only slight variations. As such, it may considered that the assumptions that have been taken for the development of the optimisation model (namely the ones related to fluid properties) are consistent, and thus the integration of the optimisation results within the finalized simulation model is overall valid.

In terms of the obtainment of optimised results, it may be verified the value for the net electricity generation for the final model is higher, which confirms the validity of the use of the adjustment scenario elaborated in the sensitivity analysis in which the thermal-to-electric efficiency is set as a value predictably lower than the one that is expected to be obtained in the final model. The obtainment of such result also has influence on the total operation costs, which has may be verified present a considerably lower value in the final configuration.

5.2. Optimisation Models for Case-study 2

In this section, the development of optimisation models for case-study 2 and the results obtained by the running of this model are presented. The development of this model takes into account the scenario defined as the most favourable in section 4.2. It is to note that a highly different formulation procedure was adopted for optimisation assessment in this case-study, owing to the presence of processes in a non-continuous mode and a thermal energy storage unit in the previously conceptualized superstructure, which obligatorily involves the variation of certain conditions through time. The elaborated WEIS scenarios took into account not only the necessity to improve fuel efficiency in intermittent kilns but also in the other energy and water-using units on the plant which are operated in a continuous mode, and thus the heat sink stream (heated air) from the constituent TES unit of these configuration was only projected to be allocated to the four combustion-based processes as each one of the combustion air streams. Such conceptual division also allows the possibility to partially separate the overall optimisation problem (which is set for the aim to minimize overall operational costs) into two problems:

- One set to minimize water and hot/ cold utilities consumption in the water system (set to be elaborated as Non-linear programming similar to one presented in section 5.1);
- One set for the minimization of natural gas consumption in the four combustion-based processes along with the time (requiring the application of the Dynamic programming methodology).

Such problem division shall ensure that optimum values are obtained for each one of the modelled sections of the overall WEIS. While the NLP model is set to be developed so to obtain values for the mass flow rate of each hot air streams that are allocated to the economisers and MED unit (in addition to the values of each water stream and equipment sizing parameter), the DP model is set to consider the limitation that it is necessary to impose to the hot air mass flow rate from each tunnel kiln (the mass flow rate allocated to the thermal process system and the remaining parts of the WEIS must not surpass the one the difference between the maximum values and the mass flow rates that were set to be allocated to the water system in the previous problem).

5.2.1. Non-linear programming (NLP) model for the Water System

Similar to case-study 1, the GEKKO Python package within Python 3.11 version software was used for the development of the proposed NLP model. Once again, the internal IPOPT software and MUMPS solver of GEKKO package were used for the running of the model.

Formulation of the Optimisation Problem

Similar to the procedure taken for case-study 1, the NLP methodology is used for the present case-study due to the formulation of the mass balance, enthalpy balance and heat transfer equations that define the system, although the objective-function is constituted by linear terms only (energy and water-related unitary costs that multiply to the respective energy and water inputs).

Since the present optimisation model has been developed on the basis of the simulation model presented in section 4.2 (namely the part of the model encompassing the water system), it is characterized by the same exact set of equations and variables that characterize the simulation model (the variables characterizing the simulation model are the decision variables of the optimisation models and the governing equations of the simulation model are formulated as equality constraints of the optimisation model). Once again, the characterization of the optimisation problem is presented in an aggregated manner in this chapter (the decision variables and constraints being presented in respective categories), with the full characterization of the problem being presented in appendix A6 (in which the respective Python code of the developed model is presented).

i) Decision Variables

The decision variables necessary to consider on the NLP model for the water system are all the mass flow rate, temperature, specific enthalpy and contaminant concentrations (namely for each one of the three contaminants in cause) that characterize each one of the water streams of the system. In addition, the hot air streams that are allocated to the economisers that are installed within the water system must also be characterized in terms of the mass flow rate and temperature/ specific enthalpy. Due to the latter requirement, the hot air streams at the outlet of each one of the two tunnel kilns considered in these case-study (whose mass flow rate, temperature and specific enthalpy are constant) are considered on the formulation of the optimisation problem. The model shall consider the splitting and mixing phenomena occurring with these streams from the origin of the two hot air streams from the respective tunnel kilns to the point in which parts of these streams are allocated (in this case, the heaters and the MED unit that are included in the water system). In Table 5-7, the decision variables and relevant inequality constraints considered for the formulation of the approached optimisation problem are characterized.

Table 5-7. Characterization of decision variables and relevant inequality constraints for the NLP model relative to case-study 2

Category	Variables
Stream-related	• Freshwater mass flow rate ($\dot{\mathrm{M}}_{\mathrm{FW}}$) • Each water stream mass flow rate ($\dot{\mathrm{M}}_{\mathrm{W}}$) • Each water stream specific enthalpy (h_{W})/ temperature (T_{W}) • Each water stream contaminant concentration (C_{W})
Sizing-related	• Heat transfer area of economisers ($\mathrm{A}_{\mathrm{Econ.}}$) • Heat transfer area of MED Effect 1 ($\mathrm{A}_{\mathrm{Eff1}}$)

Relevant Inequality Constraints		
Variable	Lower Bound	Upper Bound
Salt 1 concentration of the inlet water stream in each water-using process ($C_{W,WP,C1,in}$)	500.00	
Salt 1 concentration of the inlet water stream in each water-using process ($C_{W,WP,C1,out}$)	800.00	1000.00
Salt 2 concentration of the inlet water stream in each water-using process ($C_{W,WP,C2,in}$)	300.00	
Salt 2 concentration of the inlet water stream in each water-using process ($C_{W,WP,C2,out}$)	800.00	1000.00
Salt 3 concentration of the inlet water stream in each water-using process ($C_{W,WP,C3,in}$)	200.00	
Salt 3 concentration of the inlet water stream in each water-using process ($C_{W,WP,C3,out}$)	800.00	1000.00
Salt 1 concentration of the inlet water stream in each water-using process ($C_{W,WS,C1}$)	0.00	1000.00
Salt 2 concentration of the inlet water stream in each water-using process ($C_{W,WS,C2}$)	0.00	1000.00
Salt 3 concentration of the inlet water stream in each water-using process ($C_{W,WS,C3}$)	0.00	1000.00

ii) Constraints

The formulation of the constraints for the approached optimisation model is similar to the procedure taken for case-study 1, in which the only considered inequality constraints are the limit (minimum and maximum) values that pertain to the decision variables, with the equality constraints corresponding to all the mass balance, enthalpy balance and heat transfer equations that characterize the involved system. In Table 5-8, the equality constraints considered for the formulation of the presented optimisation problem are presented.

Table 5-8. Definition of equality constraints for case-study 2

$\dot{M}_{W.,to-be-splitted} = \sum_{i=1} \dot{M}_{W.,split,i}$	(5.25)
$h_{W.,to-be-splitted} = h_{W.,split,i}$	(5.26)
$C_{W.,to-be-splitted} = C_{W.,split,i}$	(5.27)
$\sum_{i=1} \dot{M}_{W.,to-be-mixed,i} = \dot{M}_{W.,mixed}$	(5.28)
$\sum_{i=1} (\dot{M} \cdot h)_{W.,to-be-mixed,i} = (\dot{M} \cdot h)_{W.,mixed}$	(5.29)
$\sum_{i=1} (\dot{M} \cdot C)_{W.,to-be-mixed,i} = (\dot{M} \cdot C)_{W.,mixed}$	(5.30)
$\dot{M}_{W.,in,Eff} \cdot \frac{1}{4} = \dot{M}_{TW.,Eff} + \dot{M}_{Concentrate,Eff}$	(5.31)
$q_{with.,MED} - \dot{M}_{TW.,Eff1} \cdot (h_{V,Eff1} - 418.896) = \dot{M}_{W.,in,Eff1} \cdot \frac{1}{4} \cdot (418.896 - h_{w,in,Eff})$	(5.32)
$\dot{M}_{TW.,Eff\,k-1} \cdot (h_{V,Eff1} - 418.896) = \dot{M}_{TW.,Effk} \cdot (h_{V,Effk} - 418.896) + \dot{M}_{W.,in,Effk} \cdot \frac{1}{4} \cdot (418.896 - h_{w,in,Eff})$	(5.33)
$\dot{M}_{TW.,Effect} \cdot (2675.43 - 418.896) = \dot{M}_{W.,in,Eff} \cdot \frac{1}{4} \cdot (h_{Vapour,Eff1} - 418.896)$	(5.34)
$q_{with.} = U \cdot A \cdot \left((T_{Air,in} - T_{w,out}) \cdot (T_{Air,out} - T_{w,in}) \cdot \left((T_{Air,in} - T_{w,out}) + (T_{Air,out} - T_{w,in}) \right) \cdot 0.5 \right)^{1/3}$	(5.35)

In relation to the constant values presented throughout Table 5-8, is to note:

- $\frac{1}{4}$ refers to the splitting of the water stream at the outlet of the Multi-effect distillation (MED) unit condenser to each one of the four effects;
- 418.896 (with kJ/kg units) refers to the specific enthalpy of saturated liquid water;

- 2675.43 (with kJ/kg units) refers to the specific enthalpy of saturated steam;
- 999 (with kg/ m³ units) refers to the density of liquid water.

Considering the presented decision variables and equality constraints, the present optimisation model contains 116 degrees of freedom.

iii) Objective-Function

The objective-function that shall be formulated for the present optimisation problem shall take into account the costs associated to the water system, in this case the ones referent to freshwater consumption and hot/ cold utilities consumption. For this end, the following procedure was taken based on reference unitary prices for the industrial sector:

- The unitary value of 23.66 €/GJ was considered for natural gas used as hot utility [378];
- The unitary value of 0.1459 €/kWh was considered for cold utility (with origin from electricity) [379];
- The unitary price of 1.8499 €/ m³ was considered for freshwater [380].

The objective-function formulated for this optimisation problem is presented in equation (5.36).

$$\min\left(1.8499(€/\mathrm{m^3})\cdot {}^{1}/_{999}(\mathrm{m^3/kg})\cdot \dot{\mathrm{M}}_{\mathrm{FW}}(\mathrm{kg/h}) + 23.66(€/\mathrm{GJ})\cdot \mathrm{q}_{\mathrm{Hot.Ut.}}(\mathrm{GJ/h}) + 0.1459(€/\mathrm{kWh})\cdot\frac{1}{0.95}\cdot\frac{1}{3600}(\mathrm{kWh/GJ})\cdot \mathrm{q}_{\mathrm{Cold.Ut.}}(\mathrm{GJ/h})\right)(€/\mathrm{h}) \tag{5.36}$$

Optimisation Results

The running of the optimisation model allows to obtain results associated to each one of the streams that characterize the conceptualized water system, having as basis the part of the superstructure presented in section 4.2 referent to the water-using processes, the MED unit and all recirculated water streams (as well as the hot air streams that result from the splitting and mixing of the two hot air streams at the outlet of each tunnel kiln). As such, this model is set for the obtainment of the mass flow rate, temperature and specific enthalpy associated to each water stream (and the hot air streams in question) and values associated to the effective use of freshwater and hot/ cold utilities in the water system. In Table 5-9, the optimisation results obtained for the main energy and water use indicators in the water system are presented and compared to the baseline values and the ones previously obtained throughout simulation and scenario analysis.

Table 5-9. Optimisation results for main energy and water use indicators and respective comparison

Utility/ Cost Parcel		Baseline	Scenario 2		Optimised
			With Electricity Production	With Hydrogen Production	
Water System					
Freshwater Flow Rate (m³/h)		0.861	0.419	0.460	0.527
Hot Utility Consumption (GJ/h)	**Heater 1**	0.125			
	Heater 2	0.180			
	Heater 3	0.033			
Cold Utility	**Cooler 1**	0.085			

Consumption (GJ/h)	**Cooler 2**	0.133			
	Cooler 3	0.017			
Other Indicators					
Water discharge flow rate (m^3/h)				0.062	
Treated water flow rate (m^3/h)			0.442	0.463	0.308
Hot Air from Kiln 1 to Water System Mass Flow Rate (kg/h)			5000	5000	15302.46
Hot Air from Kiln 2 to Water System Mass Flow Rate (kg/h)			5000	5000	6334.60
Overall (Water System)					
Total Operational Cost (€/h)		19.10	0.77	0.85	0.98
Total Operational Cost (k€/year)		149.47	6.06	6.66	7.63

As may be observed by the analysis of Table 5-9, the solving of the conceptualised optimisation problem converges to a point in which the use of freshwater is considerably minimized in relation to the baseline scenario and in which the hot and cold utilities consumption is null (an achievement that had already been attained for simulation scenario 2). In this prospect, it may be primarily considered that the optimisation model is robust in terms of the achievement of the proposed objective of reducing water and energy-related costs in relation to the water system. Nonetheless, it is possible to verify that freshwater flow rate for the optimised scenario is considerably higher in relation to the two simulated scenarios. Such result is in line with the obtained result for the treated water flow rate, which is considerably lower in comparison to the values obtained in the scenario analysis. As may be also verified, the optimisation problem converges to a point in which the hot air allocated from both kilns is higher. The reason for the aforementioned results may be attributed to the higher values obtained for the mass flow rate of the hot air allocated to the economisers, this is, from the total recirculated hot air from both kilns a considerable part is recirculated to the economisers rather than the MED unit, which allows a lesser production of desalinated water. In its turn, the lower quantity of desalinated water influences a lower recirculation of streams within the water system, in its turn provoking a higher consumption of freshwater.

Taking into account the aforementioned, it is possible to conclude that while the developed optimisation model is robust in respect to the considered objective (reduction of water and energy-related costs in the water system), improvements in terms of robustness may still be performed. Such improvements shall consider not only the minimization of water and energy-related costs but also the convergence of the problem to a point in which the quantity of recirculated hot air is minimized, so to furtherly allow the higher availability of hot air to be recirculated with the end to cause natural gas savings in the combustion-based processes and for electricity generation in the ORC system. In Figure 5.4, the configuration obtained with the running of the optimisation model is presented.

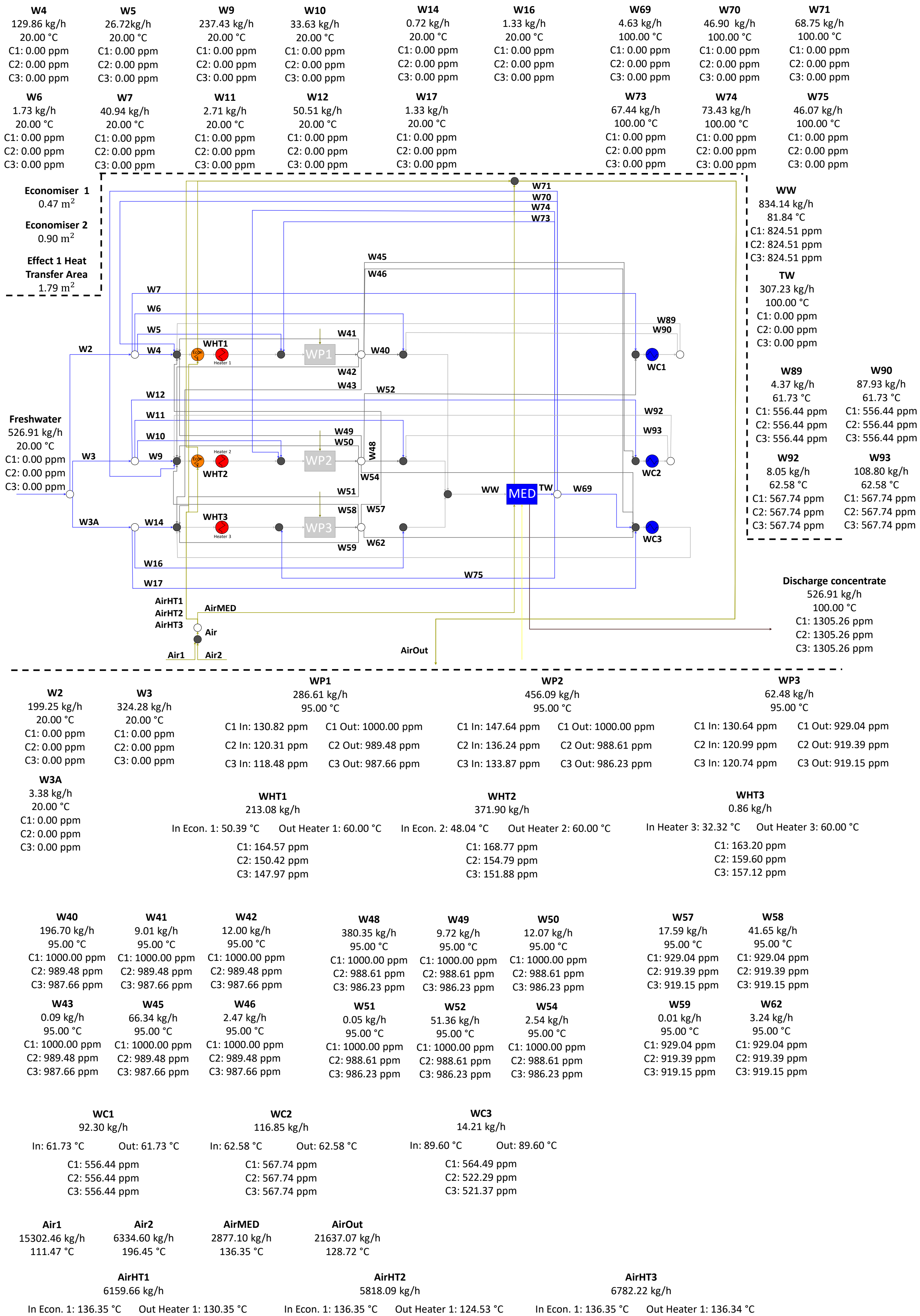


Figure 5.4. Flowsheet of the optimised Water System configuration for case-study 2

Sensitivity Analysis

The NLP model developed for the water system is set to be submitted to a sensitivity analysis, in a procedure similar to the one adopted for case-study 1. The purpose for the performance of this sensitivity analysis is mainly the improvement of the robustness of the developed model, as identified in the previous section. A total of three variations of parameters are performed in sensitivity analysis.

The present sensitivity analysis was performed by adopting a similar one-at-a-time (OAT) procedure to the one used for case-study 1, in which the value associated to a single parameter category is varied. The handling of this procedure was based on the variation of the following categories of parameters:

- The non-recirculated hot air mass flow rate from one of the kilns to the water system;
- The recirculated hot air mass flow rate from the other kiln to the water system;
- The upper bound of each salt concentration (salts 1, 2 and 3) associated to water streams (excluding the inlet and outlet streams to and from the water-using processes).

As proceeded for case-study 1, the present sensitivity analysis is set to generate an adjustment scenario that is set to potentially supplant the initial optimisation results. In this case, such supplantation is set occur through the verification of a balance between water use and hot and cold utility consumption-related benefits with the lesser input of hot air from kilns (with the aim to make possible the higher use of hot air for other applications). The characterization, results and the procedure for the alteration that follows are respectively presented in Tables 5-10 and 5.11.

Table 5-10. Sensitivity analysis results for Case-study 2 NLP model for the water system

Variables	Adjustment	Freshwater flowrate (m^3/h)	Hot utility consumption (MJ/h)	Cold utility consumption (MJ/h)	Discharge water flowrate (m^3/h)	Hot air allocated from Kiln 1 mass flowrate (ton/h)	Hot air allocated from Kiln 2 mass flow rate (ton/h)	Total operational costs (€/h)
Non-recirculated hot air from Kiln 1 (ton/h) / Recirculated hot air From Kiln 2 (ton/h)	**21.62**							
16.53	**1**	0.527				15.30	6.33	0.976
0.00	**2**	0.538				2.55		0.996
Non-recirculated hot air from Kiln 1 (ton/h) / Recirculated hot air From Kiln 2 (ton/h)	**0.00**							
16.53	**3**	0.528				21.62	5.86	0.976
0.00	**4**	0.552	78.14	1.74		21.62		2.944
Salt 1 Concentration (ppm)	**2000.00**							
Non-recirculated hot air from Kiln 1 (ton/h) / Recirculated hot air From Kiln 2 (ton/h)	**21.62**							
16.53	**5**	0.525		13.00		7.42	9.02	1.526
0.00	**6**	0.529				2.68		0.978
Salt 1 Concentration (ppm)	**2000.00**							
Non-recirculated hot air from Kiln 1 (ton/h) / Recirculated hot air From Kiln 2 (ton/h)	**0.00**							
16.53	**7**	0.537				21.62	1.65	0.993
0.00	**8**	0.536	6.21			21.62		1.138
Salt 2 Concentration (ppm)	**2000.00**							
Non-recirculated hot air from Kiln 1 (ton/h) / Recirculated hot air From Kiln 2 (ton/h)	**21.62**							

16.53	**9**	0.528				15.81	3.96	0.977
0.00	**10**	0.529				6.14		0.978
Salt 2 Concentration (ppm)	**2000.00**							
Non-recirculated hot air from Kiln 1 (ton/h) / Recirculated hot air From Kiln 2 (ton/h)	**0.00**							
16.53	**11**	0.529				21.62	4.17	0.978
0.00	**12**	0.576	38.28	0.40		21.62		1.989
Salt 3 Concentration (ppm)	**2000.00**							
Non-recirculated hot air from Kiln 1 (ton/h) / Recirculated hot air From Kiln 2 (ton/h)	**21.62**							
16.53	**13**	1.033		63.74	0.760	18.30		4.630
0.00	**14**	0.528				2.47		0.978
Salt 3 Concentration (ppm)	**2000.00**							
Non-recirculated hot air from Kiln 1 (ton/h) / Recirculated hot air From Kiln 2 (ton/h)	**0.00**							
16.53	**15**	0.527				21.62	5.91	0.976
0.00	**16**	1.033		42.75	0.696	21.62		3.730

Table 5-11. Sensitivity analysis results for Case-study 2 NLP model for the water system (Cont.)

Variables	Adjustment	Freshwater flowrate (m^3/h)	Hot utility consumption (MJ/h)	Cold utility consumption (MJ/h)	Discharge water flowrate (m^3/h)	Hot air allocated from Kiln 1 mass flowrate (ton/h)	Hot air allocated from Kiln 2 mass flow rate (ton/h)	Total operational costs (€/h)
Non-recirculated hot air from Kiln 2 (ton/h) / Recirculated hot air From Kiln 1 (ton/h)					16.53			
21.62	17	0.527				15.30	6.33	0.976
0.00	18	0.528					3.67	0.976
Non-recirculated hot air from Kiln 2 (ton/h) / Recirculated hot air From Kiln 1 (ton/h)					0.00			
21.62	19	1.033		1.53	0.562	21.56	16.53	1.976
0.00	20	0.531					16.53	0.982
Salt 1 Maximum Concentration (ppm)					2000.00			
Non-recirculated hot air from Kiln 2 (ton/h) / Recirculated hot air From Kiln 1 (ton/h)					16.53			
21.62	21	0.525		13.00		7.42	9.02	1.526
0.00	22	0.538	26.22				1.55	1.615
Salt 1 Maximum Concentration (ppm)					2000.00			
Non-recirculated hot air from Kiln 2 (ton/h) / Recirculated hot air From Kiln 1 (ton/h)					0.00			
21.62	23	0.537				21.50	16.53	0.994
0.00	24	0.528					16.53	0.977
Salt 2 Maximum Concentration (ppm)					2000.00			
Non-recirculated hot air from Kiln 2 (ton/h) / Recirculated hot air From Kiln 1 (ton/h)					16.53			
21.62	25	0.717	18.04	5.74		11.98	0.03	5.839

0.00	**26**	0.528					1.82	0.976
Salt 2 Maximum Concentration (ppm)					**2000.00**			
Non-recirculated hot air from Kiln 2 (ton/h) / Recirculated hot air From Kiln 1 (ton/h)					**0.00**			
21.62	**27**	0.530				15.45	16.53	0.980
0.00	**28**	0.546					16.53	1.010
Salt 3 Maximum Concentration (ppm)					**2000.00**			
Non-recirculated hot air from Kiln 2 (ton/h) / Recirculated hot air From Kiln 1 (ton/h)					**16.53**			
21.62	**29**	1.033		63.74	0.760	18.30		4.630
0.00	**30**	0.692	186.45	3.35			0.43	5.835
Salt 3 Maximum Concentration (ppm)					**2000.00**			
Non-recirculated hot air from Kiln 2 (ton/h) / Recirculated hot air From Kiln 1 (ton/h)					**0.00**			
21.62	**31**	0.529				13.40	16.53	0.978
0.00	**32**	1.033		57.90	0.731	0.00	16.53	4.380

By the analysis of the sequence of Tables 5-10 and 5-11, it is possible to obtain the following primary findings:

- In the majority of the performed adjustments, only small variations are verified in the analysed indicators, with relatively low freshwater consumption and hot and cold utility consumption (which reach null levels in a considerable number of the total adjustments;
- Nonetheless, in the adjustments associated to highest constrains in terms of supplied hot air (this is, in which the upper bound corresponding to the hot air allocated from one of the kilns to the water system is set as null or the upper bound for the hot air that is non-recirculated to the water system is null) it is verified either a considerably higher freshwater consumption or a higher level of consumption of either hot utility or cold utility, which provoke corresponding increases in the total operational costs (which are the cases of adjustments 4, 8, 12 and 19);
- In respect the corresponding adjustments associated to the variation of the upper bounds of concentrations of each one of the salts, it is possible to verify the inexistence of an agreement between the results throughout the comparison of several corresponding adjustments (a set of corresponding adjustments have associated lower operational costs for higher salt concentration and other sets have associated higher operational costs). As such, the consideration of the variation of the referred parameter shall be interpreted only for purposes of revise optimisation results rather than for assessment of model robustness;
- For a set of performed adjustments, it is possible to obtain a similar level of benefits in relation to the initial optimization results for reduced levels of supplied hot air from each one of the kilns (as may be verified for adjustments 2, 6, 10, 14 and 18). Such may be attributed to a tendency to maintain similar levels of water recirculation within the water system in between scenarios, and as such similar levels of water and energy use, as the defined objective for the optimisation problem is the reduction of water and energy use-related costs. In this prospect, it may be considered that the performed adjustments on the upper bounds of each one of the allocated hot air-related variables increase the robustness of the developed model in relation to the proposed objective (achieve a compromise between the reduction of total operational costs and the allocation of hot air).

Based on the previous achievements, it may be considered that although the initial optimisation model for the water system is robust in respect to the minimization of total operational costs (which is formulated as the objective-function), further adjustments may be performed to increase the overall robustness of the model in relation the objectives set as secondary (in this case, the reduction of the quantity of allocated hot air for the same level of obtained benefits). In this case, such augment of robustness related to this secondary objective is pertinent due to the fact the model has been developed only for a part of the overall conceptualized system (in this case only the water system, and not the overall WEIS). The stream allocation configuration obtained associated to the adopted configuration following sensitivity analysis (corresponding to adjustment 10) is presented in Figure 5.5.

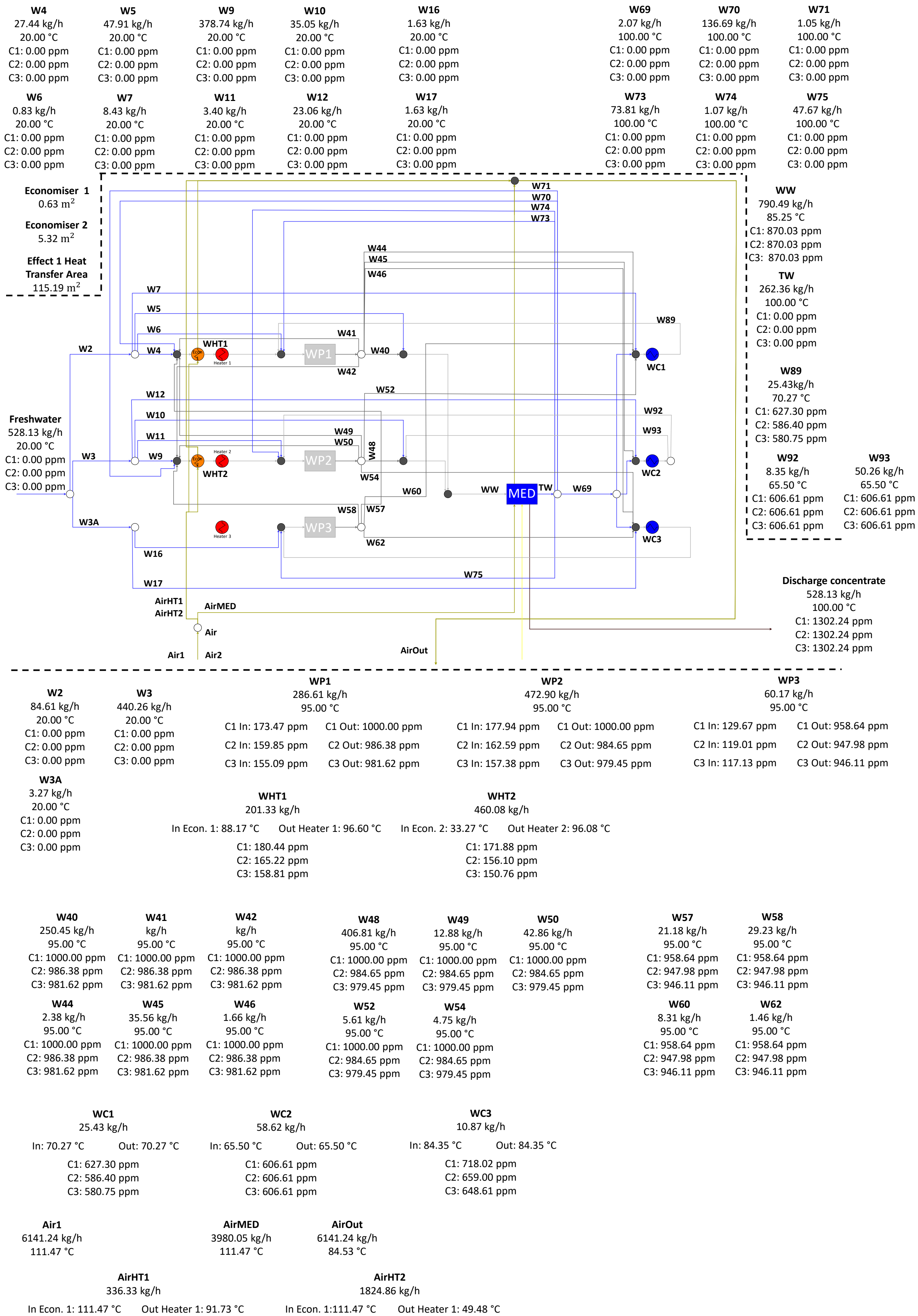


Figure 5.5. Flowsheet of the optimised Water System configuration for case-study 2

5.2.2. Dynamic programming (DP) Model for the Thermal Process System

The development of the optimisation model encompassing the thermal process system (all the combustion-based processes and the Organic Rankine cycle) is set to be developed with the *Built-in Dynamic Optimization using Annotations* OpenModelica tool. The *optimization* solver has been used and it is purposed for the running a model as a dynamic optimisation one rather than a simulation model (which in the case of this work have been running with the internal DASSL solver of OpenModelica), thus taking into account all lower and upper values defined for the variables (in the running of the model, it is ensured that these minimum and maximum values are not surpassed along the analysed time).

Formulation of the Optimisation Problem

The solving of the optimisation problem in question is set to be based on the use of the dynamic programming (DP) methodology, which has been selected due to the time-variating requirements associated to the case-study (a set of variables characterizing the system are associated to appreciable variations along operational time). While the decision variables and constraints are set to be formulated in the same manner of the previously presented optimisation models (according to a non-linear formulation, considering all the variables that characterize the streams and the mass balance, enthalpy balance and heat transfer equations), the objective-function is set to be formulated in a basis of the minimization of an absolute quantity of operational costs (the total costs associated to energy use from the start to the end of the time of analysis).

Since the present optimisation model has been developed on the basis of the simulation model presented in section 4.2 (namely the part of the model encompassing the thermal process system), it is characterized by the same exact set of equations and variables that characterize the simulation model (the variables characterizing the simulation model are the decision variables of the optimisation models and the governing equations of the simulation model are formulated as equality constraints of the optimisation model). Once again, the characterization of the optimisation problem is presented in an aggregated manner (the decision variables and constraints being presented in respective categories), with the full characterization of the problem being presented in appendix A7 (in which the Modelica code corresponding to the developed optimisation model is presented).

i) Decision Variables

The decision variables necessary to consider on the DP model for the thermal process system are all the mass flow rate, temperature/ specific enthalpy that characterize each one of the fuel, air and exhaust gas streams of the system. In Table 5-12, the decision variables, relevant inequality constraints and start values considered for the formulation of the approached optimisation problem are characterized.

Table 5-12. Decision variables, relevant inequality constraints and start values for case-study 2

Category	Variable	
Stream-related	• Natural gas flow rates ($\dot{M}_{Fuel}$)	
	• Ambient air flow rates ($\dot{M}_{Amb.Air}$)	
	• Exhaust gases flow rates ($\dot{M}_{Ex.}$)	
	• Exhaust gases specific enthalpies ($h_{Ex.}$)	
	• Hot air flow rates ($\dot{M}_{Hot\ Air}$)	
	• Hot air specific enthalpies ($h_{Hot\ Air}$)/ temperatures ($T_{Hot\ Air}$)	
	• Recirculated air flow rates ($\dot{M}_{Rec.Air}$)	
	• Recirculated air specific enthalpies ($h_{Rec\ Air}$) and temperatures ($T_{Rec\ Air}$)	
Sizing-related	• Generated electricity (Elec)	
Relevant Inequality Constraints		
Variable	**Lower Bound**	**Upper Bound**
Temperature of Mixed Gas at the outlet of the ORC ($T_{ORC,Out}$) (ºC)	70.0	
Generated electricity (Elec) (kW)	0.657	
Relevant start values		
Variable	**Start Value**	
Temperature of the PCM within the TES unit (ºC)	41.5	
Mass flow rate of the hot air stream from kiln 1 to PCM-TES unit ($M_{Hot\ Air,kiln\ 2,TES}$) (kg/h)	5000	

In respect to the presented setup for relevant inequality constraint and start values, the following aspects must be pointed out:

- The generated electricity was defined as the output from the ORC already discounting electricity consumption in the ORC pump but not the electricity that is set to be used for the operation of the MED unit, so a lower limit has been defined representing the latter (0.657 kW);
- The start value for the PCM temperature has been defined as the temperature of the inlet ambient air in the kilns (41.5 ºC).

ii) Constraints

In a similar manner to the previously developed optimisation models, the present optimisation model has been created bearing in the mind the definition of inequality constraints as the lower and upper bounds for each one of the system variables only. The equality constraints characterizing this model consists in the mass balance, enthalpy balance and heat transfer equations that define the variations in-between each mass flow rate, specific enthalpy and temperature variables, in addition to the equations characterizing the storage of thermal energy within the PCM-TES unit (which must be elaborated as time-dependent equations, as according to the specific requirements of this case study). In Table 5-13, the equality constraints considered for the formulation of the presented optimisation problem are presented in an aggregated manner.

Table 5-13. Definition of equality constraints for case-study 2 (Thermal Process System)

Thermal Process System (Stream Recirculation)		
	$\dot{M}_{Comb.Air} = \dot{M}_{Rec.Air} + \dot{M}_{Amb.Air}$	(5.37)
	$\dot{M}_{C.Air} \cdot h_{Comb.Air} = \dot{M}_{Rec.Air} \cdot h_{Recyc.Air} + \dot{M}_{Amb.Air} \cdot h_{Amb.Air}$	(5.38)
	$\dot{M}_{Fuel} + \dot{M}_{C.Air} = \dot{M}_{Ex.}$	(5.39)
	$\dot{M}_{Fuel} \cdot AF = \dot{M}_{C.Air}$	(5.40)
	$AF \cdot LHV_{NG} = AF_{Baseline} \cdot LHV_{Fuel}$	(5.41)
	$LHV_{Fuel} = Y_{NG} \cdot LHV_{NG} + Y_{H_2} \cdot LHV_{H_2}$	(5.42)
	$\dot{M}_{gas,in,ORC} \cdot \left(h_{gas,in,ORC} - h_{gas,out,ORC}\right) \cdot 0.0422 = Elec \cdot 3600$	(5.43)
Thermal Energy Storage-Related		
Charge Phase	$\frac{dT_{PCM}}{dt} = \frac{0.15}{890 \cdot C_{PCM}} \cdot \frac{1}{(r_{ext} + r_{int}) \cdot 0.5} \cdot \left(\left(\frac{T_{PCM,N} - T_{PCM,1}}{r_{ext} - r_{int}}\right) + \left(\frac{T_{PCM,N} - 2 \cdot T_{PCM} + T_{PCM,1}}{(r_{ext} - r_{int})^2}\right)\right)$	(5.44)
Discharge Phase	$\frac{dT_{PCM}}{dt} = \frac{0.15}{890 \cdot C_{PCM}} \cdot \frac{1}{(r_{ext} + r_{int}) \cdot 0.5} \cdot \left(\left(\frac{T_{PCM,1} - T_{PCM,N}}{r_{ext} - r_{int}}\right) + \left(\frac{T_{PCM,1} - 2 \cdot T_{PCM} + T_{PCM,N}}{(r_{ext} - r_{int})^2}\right)\right)$	(5.45)
	$C_{PCM} = \frac{225000}{(2 \cdot 3.1416)^{0.5} \cdot 0.1626} \cdot \exp\left(\frac{-(T_{PCM} - 72)^2}{2 \cdot 0.1626^2}\right) + 2200$	(5.46)

In relation to the constant values presented throughout Table 5-13, is to note:

- 0.0422 refers to the thermal-to-electric conversion efficiency associated to the Organic Rankine cycle (ORC);
- 3600 (with kJ/kWh units) refers to the factor of conversion of kWh to kJ energy units;
- 0.15 (with W/(m.ºC) units) refers to the thermal conductivity of the considered PCM;
- 890 (with kg/m^3 units) refers to the density of the considered PCM;
- 225000 (with J/kg units) refers to the latent enthalpy associated to the melting/ solidification of PCM (as required as a parameter on the apparent specific heat capacity determination equation);
- 3.1416 is an approximation of pi;
- 0.1626 (with ºC units) refers to the temperature constant for the PCM microstructure (as required as a parameter on the apparent specific heat capacity determination equation);
- 72 (with ºC units) refers to lower bound for the temperature range of the melting/ solidification phase of the PCM (as required as a parameter on the apparent specific heat capacity determination equation);
- 2200 (with J/(ºC.kg) units) refers to the specific heat capacity for the solid phase of the PCM (as required as a parameter on the apparent specific heat capacity determination equation);

Since the present dynamic optimisation model is developed as a simulation-based optimisation model, the number of degrees of freedom is zero.

iii) Objective-Function

In a similar manner to the previously developed models, the objective-function set to be defined for the present optimisation model shall reflect the minimisation of a determinate function related to operational costs. For the previous developed models, this function was defined in basis of the minimisation of the summation of all energy and water costs per unit of operational time (in those cases in an hourly basis, €/h). The change of the paradigm of a steady-state perspective to a dynamic-based perspective brings different requirements to define the function to minimize, as the values associated to variables that are involved in the computation of these costs (mass flow rates of natural gas streams and generated electricity) effectively vary along the operational time. In this prospect, the set-to-be-defined objective-function must be enunciated based on the following procedure typically adopted for dynamic programming:

- Minimization of operational costs per each instant of time (corresponding to the Lagrange Term);
- Minimization of operational costs in the final time instant (corresponding to the Mayer Term).

The adoption of one or the other method leads to similar results, as these are enunciated with the objective to ensure that the total operational costs in the final time instant (given in absolute € units) are the least possible. In a similar manner to the previously developed models, the following procedure was taken based on the aforementioned reference unitary prices for the industrial sector. The objective-function formulated for the present optimisation problem is presented in the sequence of equations (5.47) – (5.49). The aforementioned second method (using the Mayer Term) was used for the described purpose (minimization of the total operational costs in the final time instant of analysis).

$$\mathrm{OBJ} = \left(\left(23.66(€/\mathrm{GJ}) \cdot 0.0453(\mathrm{GJ/kg}) \cdot \dot{\mathrm{M}}_{\mathrm{NG}}(\mathrm{kg/h}) - 0.1459(€/\mathrm{kWh}) \cdot \mathrm{Elec}_{\mathrm{Eff}}(\mathrm{kWh/h})\right) \cdot \frac{1}{3600}(\mathrm{s/h})\right)(€/\mathrm{s}) \tag{5.47}$$

$$\mathrm{OBJ}(€/\mathrm{s}) = \left(\frac{\mathrm{d}}{\mathrm{dt}}\left(\mathrm{OBJEff}(€)\right)\right)(€/\mathrm{s}) \tag{5.48}$$

$$\min\left(\mathrm{OBJEff}\ (\mathrm{t} = 151200\ \mathrm{s})\ (€)\right), \mathrm{OBJEff}\ (\mathrm{t} = 0\ \mathrm{s}) = 0\ € \tag{5.49}$$

Optimisation Results

The results obtained by the running of the presented dynamic optimisation model must be analysed in a substantially different manner in comparison to the previously developed models, as the values obtained for each variable of interest vary according to time. As such, the plot of each one of the variables that characterize the thermal process system must be presented for the further analysis of optimisation results. In a similar manner to the previously presented models, the variables of interest to be analysed are the mass flow rate and temperature/

specific enthalpy that characterize each one of the system streams (in this case these are only gas streams). In this model, the temperature of the PCM within the TES unit (PCM-based heat exchanger) must also be analysed. The optimisation results relative to the determination of each energy and water use indicators are presented in Table 5-14. The optimisation results in respect to specific system variables are presented in the sequence of Figures 5.6 – 5.9.

Table 5-14. Optimisation results for the main energy and water use indicators and its comparison with initial and previously obtained values for the case-study 2 thermal process system (one cycle corresponds to 42 hours)

Utility/ Cost Parcel		Baseline	Scenario 2		Optimised
			With Electricity Production	With Hydrogen Production	
Thermal Process System					
Natural Gas Flow Rate (kg/cycle)	Kiln 1	5355.00	4872.45	4872.45	4839.79
	Kiln 2	5044.20	3992.10	3931.88	3941.36
	Kiln 3	334.29	324.27	324.27	319.59
	Kiln 4	1266.05	1245.40	1245.40	1234.03
Net Generated Electricity (kWh/cycle)			1437.81		1588.61
Overall (Thermal Process System)					
Total Operational Cost (k€/cycle)		12.80	10.92	11.07	10.80
Total Operational Cost (M€/year)		2.38	2.03	2.06	2.01

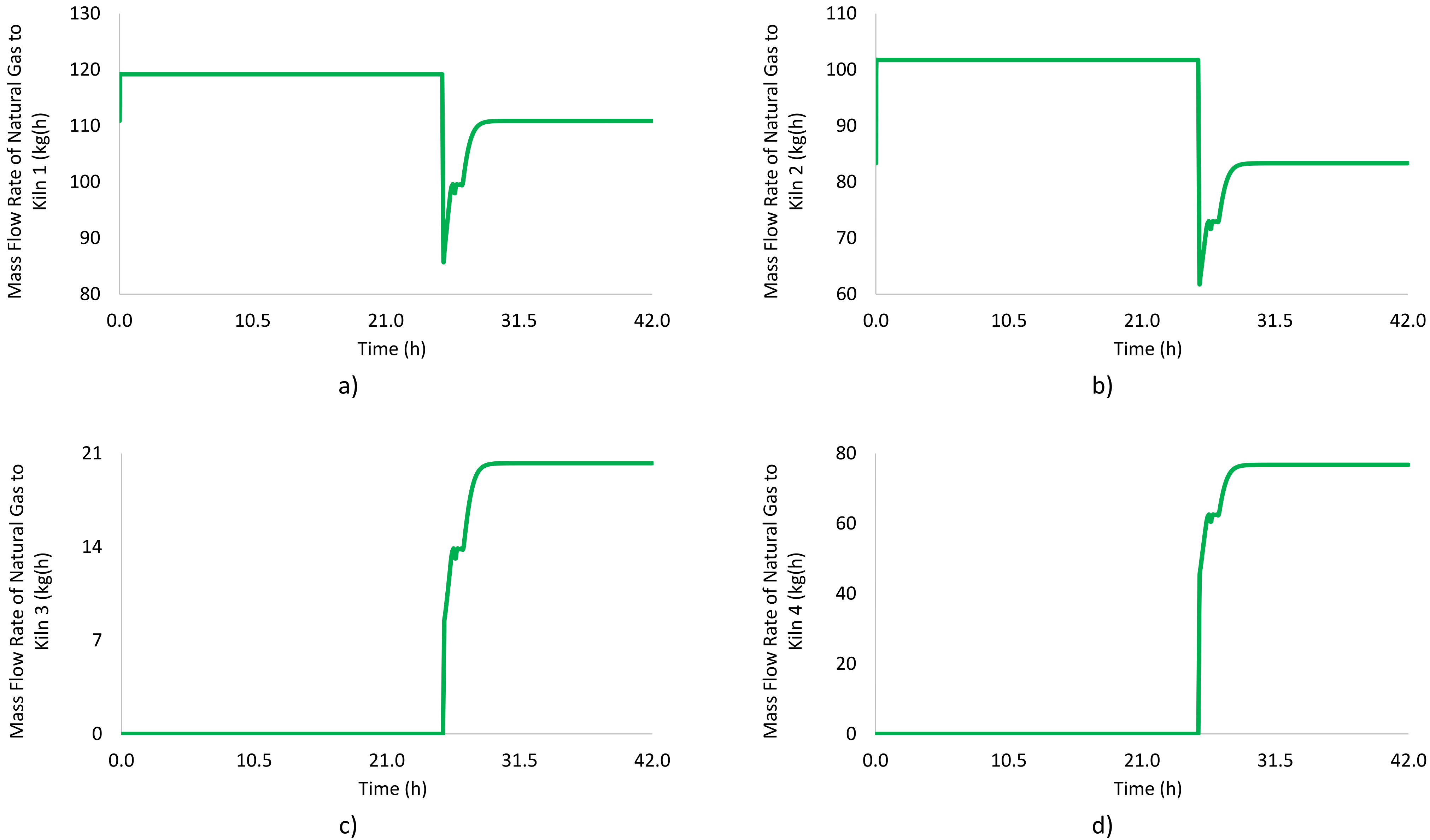


Figure 5.6. Optimisation results along time for the mass flow rate of natural gas of a) Kiln 1, b) Kiln 2, c) Kiln 3 and d) Kiln 4

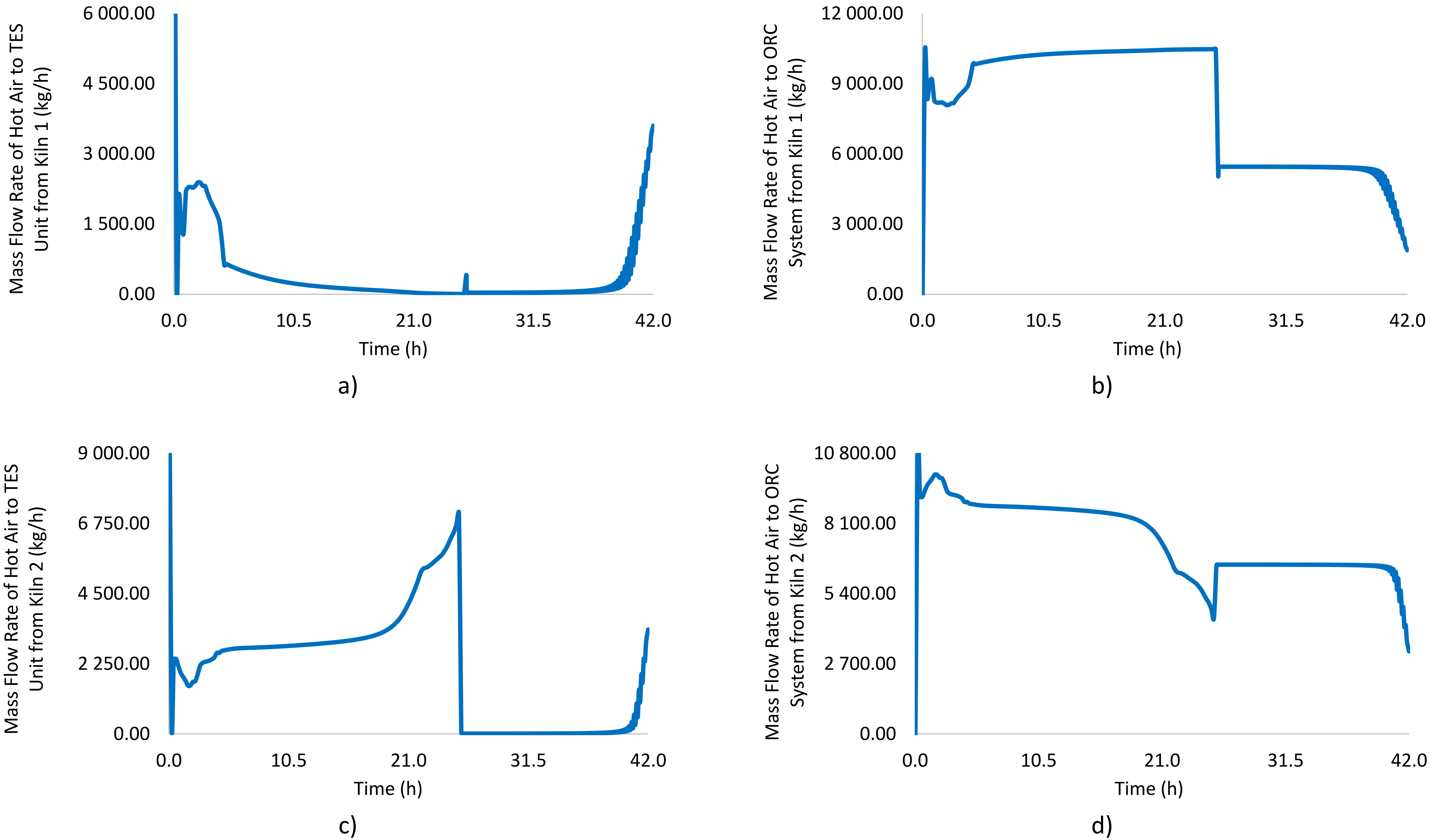
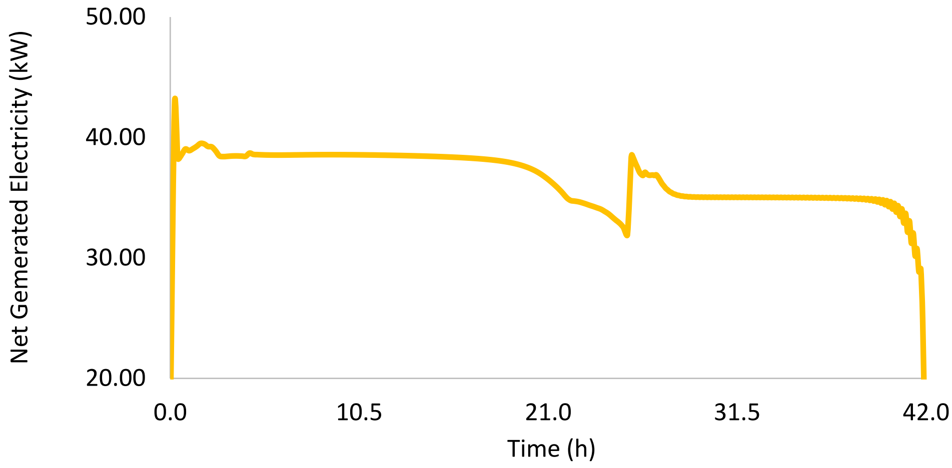
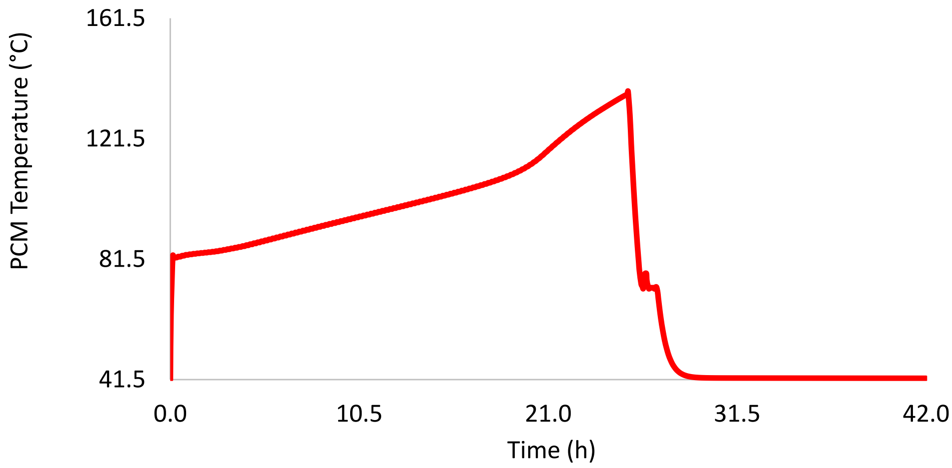


Figure 5.7. Optimisation results along time for the mass flow rate of hot air form a) Kiln 1 to TES Unit, b) Kiln 1 to ORC System, c) Kiln 2 to TES Unit, d) Kiln 2 to ORC System



a)



b)

Figure 5.8. Optimisation results along time for the mass flow rate of hot air form a) Generated electricity, b) Temperature of the PCM inside the PCM-based heat exchanger

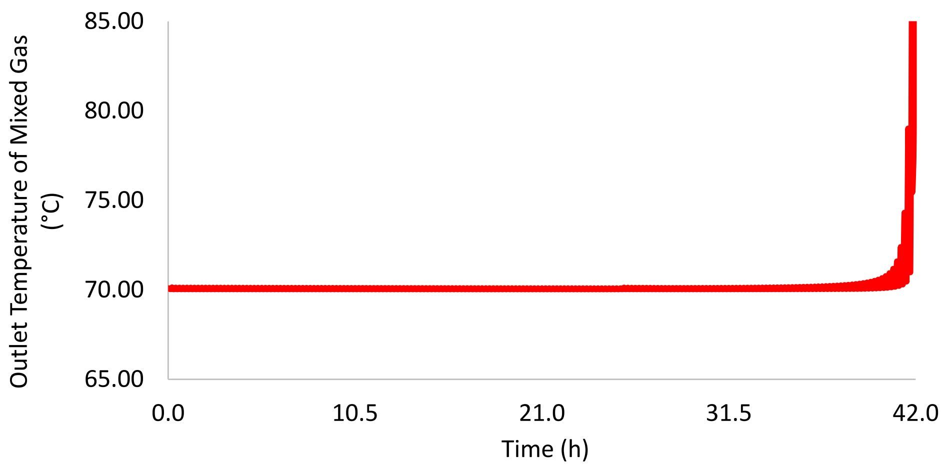


Figure 5.9. Optimisation results along time for the temperature of the mixed gas at the outlet of the HRSG unit included in the ORC system

From the observation of the results presented in Table 5-14, the following affirmations may be performed:

- The solving of the optimisation problem converges to a point in which the total operational costs (the summation of each one of the energy-related cost parcels) is considerably lower than the corresponding baseline value and the value obtained for the previously elaborated scenario analysis;
- For all the case-study combustion-based processes (kilns), the natural gas consumption is significantly lower than the corresponding values for the baseline scenario and the scenario analysis;
- The generated electricity in the ORC system is also considerably higher, thus producing higher savings related to the use of electric energy.

At the light of the aforementioned verifications, it may be considered that the solving of the optimisation problem has been successful for the achievement of the proposed objective of assessing potential energy use-related improvements.

The analysis of the time-varying results for the approached system variables may be conveniently proceeded through its division in two parts:

- Analysis of the results during the charge phase (first 25.5 hours of analysed time);
- Analysis during the discharge phase (the remaining 16.5 hours).

In relation to the charge phase:

- It is possible to verify by the analysis of Figure 5.6 that the mass flow rate of natural gas at the inlet of each kiln is constant throughout all the analysed time in question, as the temperature of combustion air at the inlet of each kiln is set as the value corresponding to the scenario analyses setups. For kilns 3 and 4, the natural gas flow rate is null since these are intermittent kilns that do not operate at charge phase. The aforementioned results are identical to the ones obtained by the corresponding simulation, as it is supposed to occur;
- The most crucial aspect of the optimisation procedure during the discharge phase is the allocation of the hot air streams at the outlet of kilns 1 and 2, which are the ones whose mass flow rate must be varied with the aim to obtain the minimized operational cost at the end of the analysed time (according to the formulation of the objective-function);
- By the analysis of Figure 5.7 – a) and c), it is possible to verify a slight increase of the quantity of hot air allocated from kiln 1 to the TES unit followed by two moments of gradual decrease and a gradual increase of the quantity of hot air from kiln 2. Such may be attributed to an adopted tendency OpenModelica *optimization* solver to converge to a point in which the stored enthalpy within the PCM-TES unit is increased (which may be observed by the increase of the PCM temperature in Figure 5.8 – b)), which may achieved through the supply of the hot air stream with a higher temperature (in this case the one from kiln 2) in higher quantities. Since the moment in which a constant PCM temperature is not achieved (corresponding to the thermal equilibrium between the heat source and the stored material), it is not verified the starting of a decrease of the supply of this hot air in a determinate instant. In its turn, the gradual decrease of the supply of the hot air from kiln 1

may be attributed to a tendency of the results to converge to a point in which the hot air from kiln 2 is allocated in its place, owing to its higher temperature;

- In relation to the generated electricity, it is possible to observe in Figure 5.8 – a) a relative stagnation for the first hours of analysis (roughly the first 19 hours), with a gradual decrease from that point to the end of the charge phase. The first moment (of relative stagnation) may be interpreted as assuming an equilibrium between the supplied hot air from kilns 1 (which is gradually increasing) and 2 (which is decreasing). The second moment (of gradual decrease) may be attributed to the verifiable decrease of the quantity of hot air from kiln 2 to the ORC system from the 19 hours instant onwards (which is directed to the TES unit instead);
- The temperature of the mixed gas at the outlet of the ORC is roughly maintained at the 70.0 ºC (the defined lower limit), which may be attributed to the convergence of the solver for the maximization of generated electricity for the whole analysis time.

In respect to the discharge phase:

- It is possible to verify that the mass flow rate of the natural gas in each kiln is effectively lower than the corresponding baseline and the simulation scenarios (taking the natural gas flow rate to kiln 1, while for the simulation scenarios it attains a level above 90.0 kg/h for the optimised scenario it is decreased to a much lower value on the first moments of the discharge phase), as it is expected to occur due to the relatively superior temperature of the combustion air that is preheated through the withdrawal of enthalpy from the TES unit;
- In its turn, the mass flow rates of the hot air streams allocated to the TES unit take approximately null values, which is an expected result as the supply of these streams signifies the supply of enthalpy to the TES unit, which must not be verified during the discharge phase.

Overall, it may be affirmed that the developed DP model is valid in the aspects that it is able to achieve the desired objective (considerable savings in operational costs associated to natural gas and electricity use) and the expected occurrence of physical phenomena (as detailed afore). Nonetheless, the model subsists on the flowing drawbacks in terms of result obtainment:

- The mass flow rate of the hot air streams allocated to the TES unit in the last hours of the analysed time present higher than null values, which by the reasons pointed afore it is not supposed to be verified;
- By the same set of reasons associated to the previous point, the mass flow rate of the hot air streams allocated to the ORC system present considerably low values (for the same time interval);
- In a further analysis attributed to the same set of reasons associated to the previous point, The temperature of the mixed gas at the outlet of the ORC presents an exacerbated increase from the 37 hours instant to the end of the discharge phase;

In this prospect, it may be considered that although the model is able to produce optimisation results that may be used to be integrated with the simulation model (essentially for the charge phase), only such integration is able the obtainment of final results to be used for further post-processing assessment.

Sensitivity Analysis

In a similar manner to the previously presented models, the developed DP model is set to be submitted to a sensitivity analysis, with a similar one-at-a-time (OAT) procedure being set to be used. The objective of such analysis is the same as the previously elaborated ones, in which the robustness of the model at the light of the obtainment of optimal results is set to be assessed. The results to be evaluated shall be the ones calculated in a basis of the considered 42-hour cycle, rather than an hourly basis, as proceeded for the previous steps elaborated in the scope of this model.

The handling of this procedure was based on the variation of the following categories of parameters:

- The start values for the mass flow rate of the hot air allocated from the kilns to the TES unit;
- The mass flow rate of the hot air recirculated as preheated combustion air in each one of the kilns;
- The thermal-to-electric conversion efficiency associated to the ORC.

The performed variations on the model parameters and the respective results are presented in the sequence of Tables 5-15 – 5-20.

Table 5-15. Characterization of the proceeded adjustment and obtained results (Adjustment 1)

Characterization					
Start value for the mass flow rate of the hot air stream allocated from kiln 1 to the TES Unit ($M_{Hot\ Air,kiln\ 1,TES}$) is varied, with the following three values being set: • 500.00 kg/h (Alteration 1.1); • 1000.00 kg/h (Alteration 1.2); • 3000.00 kg/h (Alteration 1.3).					
Previous Results Scenario		Initial Optimised Scenario			
Results					
Indicator		**Previous Results**	**Adjustment 1.1**	**Adjustment 1.2**	**Adjustment 1.3**
Thermal Process System					
Natural Gas Flow Rate (kg/cycle)	**Kiln 1**	4839.79	4827.98	4825.89	4831.57
	Kiln 2	3941.36	3930.55	3928.58	3933.68
	Kiln 3	319.59	312.91	311.64	314.70
	Kiln 4	1234.03	1219.19	1216.57	1223.71
Net Generated Electricity (kWh/cycle)		1588.61	1508.02	1608.87	1564.15
Overall (Thermal Process System)					
Total Operational Cost (k€/cycle)		10.80	10.76	10.74	10.77
Total Operational Cost (M€/year)		2.01	2.00	2.00	2.01
Procedure for the further alteration					
Adjustment 1.2 supplants the initial considered values.					

Table 5-16. Characterization of the proceeded adjustment and obtained results (Adjustment 2)

Characterization					
Start value for the mass flow rate of the hot air stream allocated from kiln 2 to the TES Unit ($M_{Hot\ Air,kiln\ 2,TES}$) is varied, with the following three values being set: • 4500.00 kg/h (Alteration 2.1); • 4800.00 kg/h (Alteration 2.2); • 5100.00 kg/h (Alteration 2.3).					
Previous Results Scenario		Adjustment 1.2			
Results					
Indicator		**Previous Results**	**Adjustment 2.1**	**Adjustment 2.2**	**Adjustment 2.3**
Thermal Process System					
Natural Gas Flow Rate (kg/cycle)	**Kiln 1**	4825.89	4832.29	4835.68	4765.10
	Kiln 2	3928.58	3934.52	3937.53	3872.90
	Kiln 3	311.64	315.39	317.17	277.15
	Kiln 4	1216.57	1224.60	1228.87	1140.22
Net Generated Electricity (kWh/cycle)		1608.87	1594.15	1606.85	1378.23
Overall (Thermal Process System)					
Total Operational Cost (k€/cycle)		10.74	10.77	10.78	10.53
Total Operational Cost (M€/year)		2.00	2.01	2.01	1.96
Procedure for the further alteration					
Adjustment 2.3 supplants the initial considered values.					

Table 5-17. Characterization of the proceeded adjustment and obtained results (Adjustment 3)

Characterization			
Start value for the mass flow rate of the hot air stream allocated from kiln as combustion air ($M_{6,AA}$) is varied from 5000 kg/h (charge phase) and 10000 kg/h (discharge phase) to 12000 kg/h.			
Previous Results Scenario		Adjustment 2.3	
Results			
Indicator		**Previous Results**	**Adjustment 3**
Thermal Process System			
Natural Gas Flow Rate (kg/cycle)	**Kiln 1**	4765.10	4491.19
	Kiln 2	3872.90	3936.21
	Kiln 3	277.15	316.43
	Kiln 4	1140.22	1226.92
Net Generated Electricity (kWh/cycle)		1378.23	852.03
Overall (Thermal Process System)			
Total Operational Cost (k€/cycle)		10.53	10.52
Total Operational Cost (M€/year)		1.96	1.96
Procedure for the further alteration			
Adjustment 3 supplants previous results.			

Table 5-18. Characterization of the proceeded adjustment and obtained results (Adjustment 4)

Characterization			
Start value for the mass flow rate of the hot air stream allocated from kiln as combustion air ($M_{13,AA}$) is varied from 5000 kg/h (charge phase) and 10000 kg/h (discharge phase) to 10000 kg/h.			
Previous Results Scenario		Adjustment 3	
Results			
Indicator		**Previous Results**	**Adjustment 4**
Natural Gas Flow Rate (kg/cycle)	**Kiln 1**	4491.19	4493.45
	Kiln 2	3936.21	3470.81
	Kiln 3	316.43	317.67
	Kiln 4	1226.92	1230.19
Net Generated Electricity (kWh/cycle)		852.03	1397.65
Overall (Thermal Process System)			
Total Operational Cost (k€/cycle)		10.52	9.95
Total Operational Cost (M€/year)		1.96	1.85
Procedure for the further alteration			
Adjustment 4 supplants previous results.			

Table 5-19. Characterization of the proceeded adjustment and obtained results (Adjustment 5)

Characterization			
Value for the thermal-to-electric efficiency associated to the ORC system is varied from 4.22% to 1.50%.			
Previous Results Scenario		Adjustment 4	
Results			
Indicator		**Previous Results**	**Adjustment 5**
Thermal Process System			
Natural Gas Flow Rate (kg/cycle)	**Kiln 1**	4493.45	4480.88
	Kiln 2	3470.81	3456.20
	Kiln 3	317.67	308.91
	Kiln 4	1230.19	1210.15
Net Generated Electricity (kWh/cycle)		1397.65	470.47
Overall (Thermal Process System)			
Total Operational Cost (k€/cycle)		9.95	10.02
Total Operational Cost (M€/year)		1.85	1.87
Procedure for the further alteration			
Adjustment 5 supplants previous results, owing to lower fuel consumption in kilns.			

Table 5-20. Characterization of the proceeded adjustment and obtained results (Adjustment 6)

Characterization			
Value for the thermal-to-electric efficiency associated to the ORC system is varied from 4.22% to 6.00%.			
Previous Results Scenario		Adjustment 4	
Results			
Indicator		**Previous Results**	**Adjustment 6**
Natural Gas Flow Rate (kg/cycle)	**Kiln 1**	4493.45	4491.75
	Kiln 2	3470.81	3469.04
	Kiln 3	317.67	316.82
	Kiln 4	1230.19	1227.81
Net Generated Electricity (kWh/cycle)		1397.65	1655.85
Overall (Thermal Process System)			
Total Operational Cost (k€/cycle)		9.94	9.90
Total Operational Cost (M€/year)		1.85	1.84
Procedure for the further alteration			
Adjustment 6 is set as an alternative to Adjustment 5.			

By the analysis of the sequence of Tables 5-15 – 5-20, it is possible to perform the following primary verifications:

- For the alterations in respect to the model parameters proper (adjustments 1 and 2, this is, the ones which are no related to the pre-defined setup of start values for stream allocation-related variables), the overall variations in terms of the analysed energy use indicators (fuel consumption and electricity consumption) are not significant. In this sense, it may be considered that the DP model as initially conceived had been robust in relation to the defined objective, although improvements in such aspect may had still be performed;
- In relation to the adjustment related to stream allocation-related parameters (adjustments 3 and 4), it is verified that a further re-assessment of the initially defined values may be performed so to obtain higher levels of total operation cost reduction. The most significant benefit with these two adjustments is effectively the reduction of the natural gas consumption on the kilns operating in continuous mode (kilns 1 and 2), which overall provokes the decrease on total operational costs. On the other hand, the natural gas consumption on the intermittent kilns (kilns 3 and 4) increases from adjustment 2 to 3 and 3 to 4 (which is expected due to the decrease of the availability of hot air to be supplied to the PCM-TES unit). The obtained value for the net generated electricity at the end of the analysis time (42 hours) has been differentially affected, with the adjustment on the mass flow rate of the hot air recirculated from kiln 1 (adjustment 3) producing a lower level of net generated electricity and the one for the hot air from kiln 2 (adjustment 4) producing a higher level. This higher level of net generated electricity may be attributed to a more effective allocation of the hot air to the ORC system in adjustment 4. As already have been established in the previous section, the *optimization* solver may allow a convergence of the solution to a point in which a part of the hot air from both kilns is allocated to the TES unit in the discharge phase (as such, adjustment 4 may correspond to a solution in which the hot air is more effectively allocated to the ORC system as it is set to be more conveniently allocated);
- In relation to the adjustments related to thermal-to-electric energy conversion efficiency of the ORC system (adjustment 5 and 6), it is verified that only slight variations occur for natural gas consumption, with the net generated electricity being the energy use-related indicator with the highest variation (in this case, decrease and increase for respectively adjustments 5 and 6). As such, it may be affirmed that adjustments performed for the ORC thermal-to-electric conversion efficiency provoke essentially a corresponding variation on the net generated electricity, not affecting the remaining indicators. The obtainment of such levels for each one of the referred indicators may be attributed to similar levels of allocation of hot air in each instant of time, this is, the solution converges to the similar mass flow rates of each one of the hot air streams from the kilns to the TES unit in adjustments 4, 5 and 6.

Attending to the aforementioned verifications, it may be concluded that the present optimisation model as initially setup may be considered robust. The adjustments performed for the parameters proper (which in this case consist in start values for system variables) do not cause considerable variations in respect to the analysed indicators. Nevertheless, it is verified that for stream allocation-related parameters that had been initially set as pre-defined values (not being considered to variate according to time in a perspective of dynamic optimisation), further adjustments shall be performed for the purpose of obtainment of improvements in terms of energy use indicators. In general, the developed model may be considered robust in respect to the defined objective. In a perspective of advanced analysis, it may be of interest to analyse the potential associated to the setup of the model considering the variation of the parameters initially set with pre-defined values along with time, so to attain a higher robustness of the model in terms of the consideration of a higher number of potential scenarios (associated to the varying allocated hot air streams mass flow rates).

At the light of the presented observations, the configuration obtained by adjustment 5 is set as the one to be considered for further step of integration within the simulation model. Similarly to the procedure adopted for the NLP model of case-study 1, adjustment 5 is the one in which it is obtained a compromise between the highest possible reduction of total operational costs and the insurance of the obtainment of the most coherent results associated to electricity generation, in which the thermal-to-electric energy conversion efficiency is considerably decreased so to ensure that the definitive solution is the one associated to the minimum level of total operational costs. The revised optimisation results in respect to specific system variables are presented in the sequence of Figures 5-10 – 5-13.

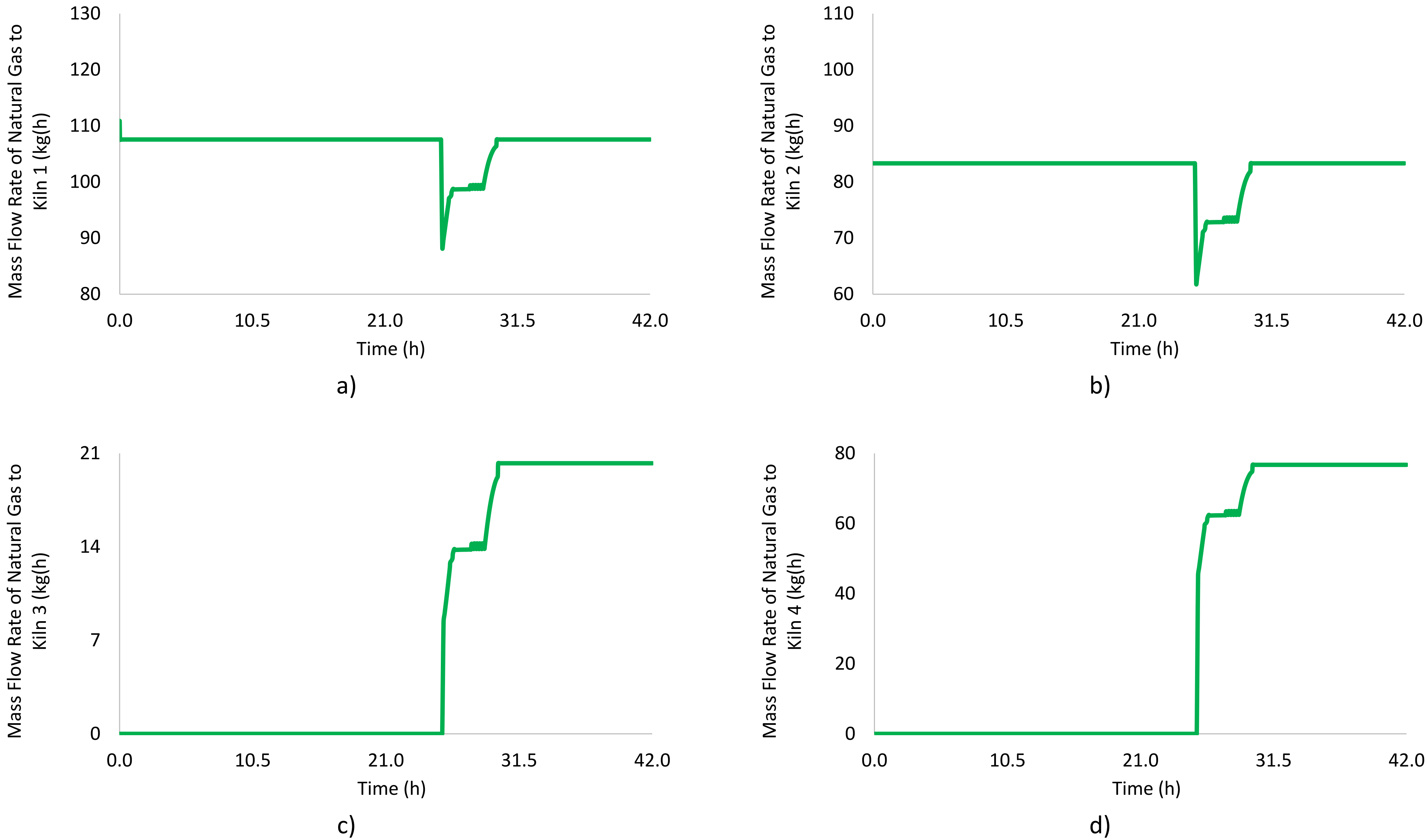


Figure 5.10. Revised optimisation results along time for the mass flow rate of natural gas of a) Kiln 1, b) Kiln 2, c) Kiln 3 and d) Kiln 4

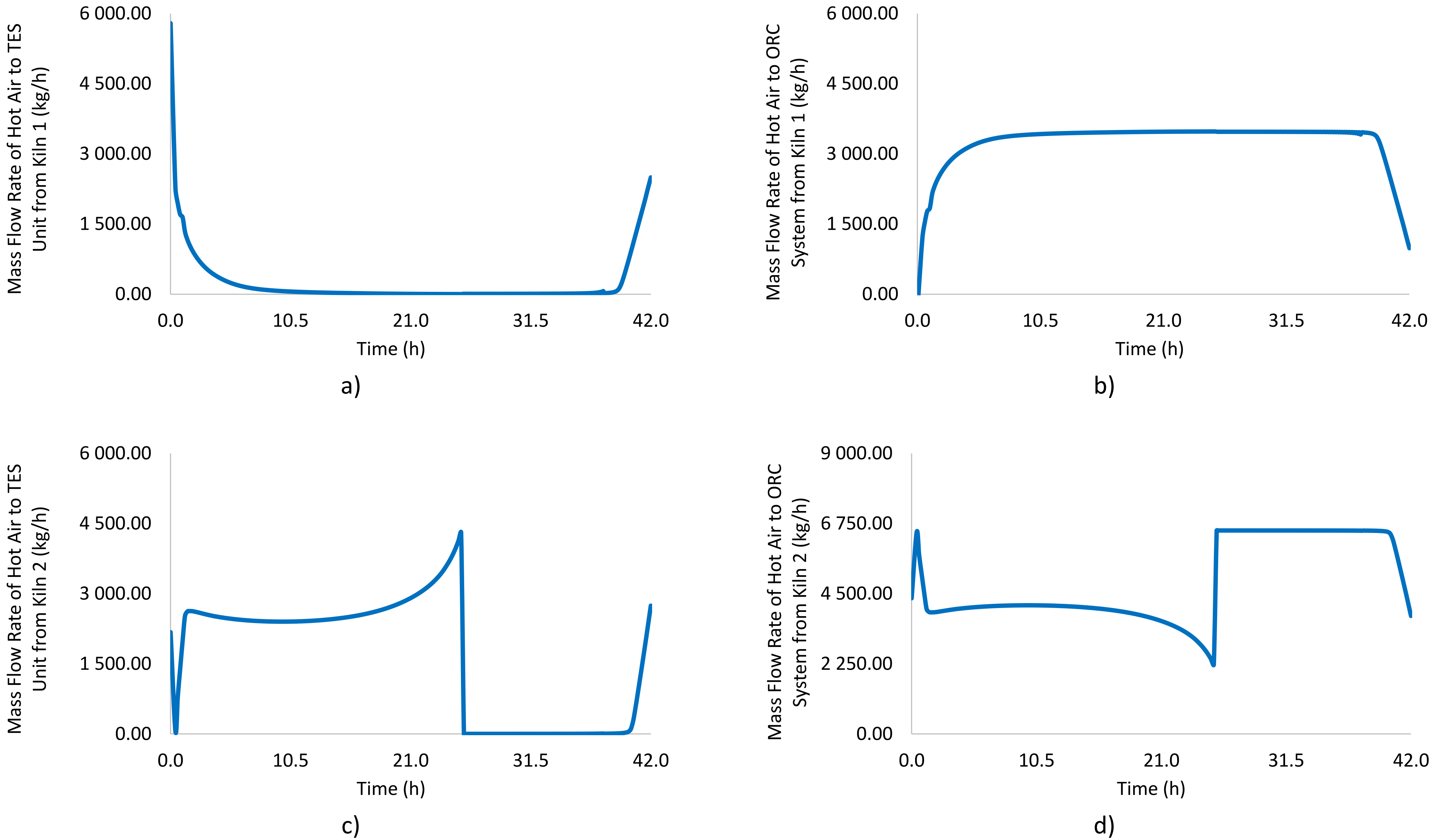
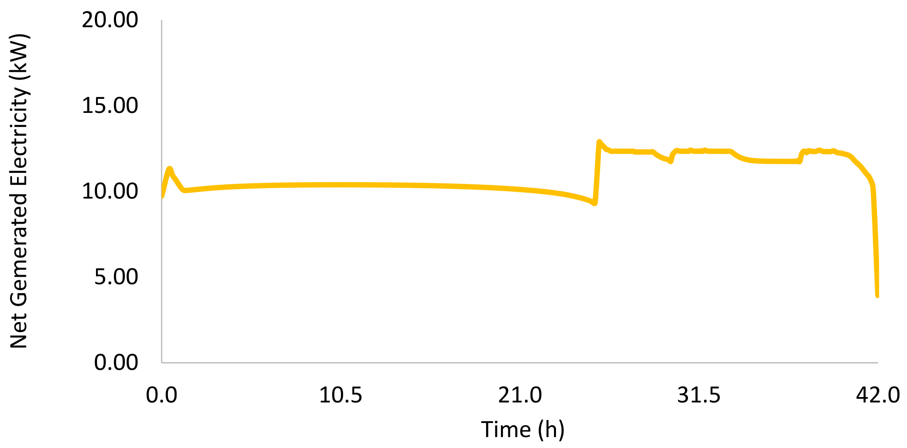
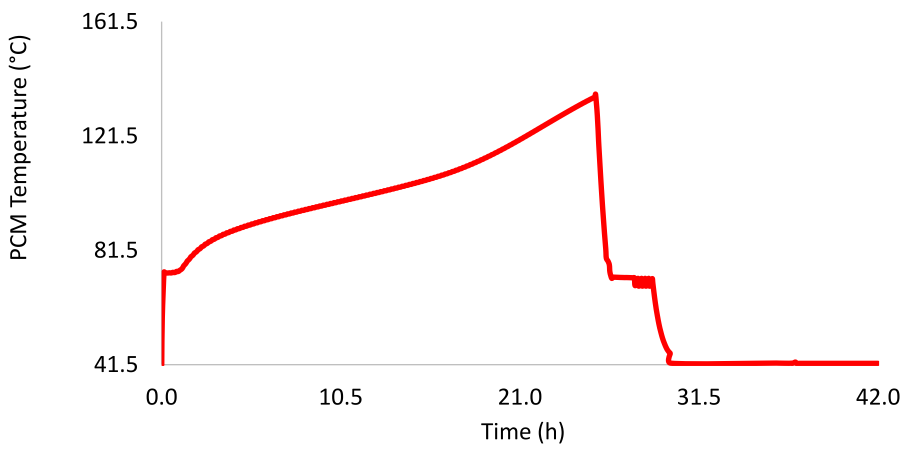


Figure 5.11. Revised optimisation results along time for the mass flow rate of hot air form a) Kiln 1 to TES Unit, b) Kiln 1 to ORC System, c) Kiln 2 to TES Unit, d) Kiln 2 to ORC System



a)



b)

Figure 5.12. Revised optimisation results along time for a) Generated electricity, b) Temperature of the PCM inside the PCM-based heat exchanger

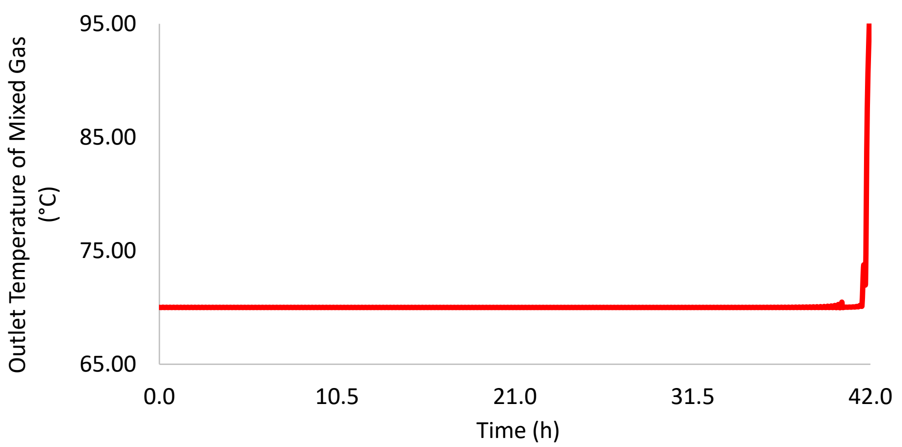


Figure 5.13. Revised optimisation results along time for the temperature of the mixed gas at the outlet of the HRSG unit included in the ORC system

Integration with the Simulation Model

The set of the two optimisation models presented throughout the presented section have been conjointly developed with the aim to assess the minimum possible water and energy input in the conceptualized system at the end of a determinate interval of time (which in this case is set as the end of an enthalpy charge/ discharge cycle). In the case of the optimisation model presented in section 5.2.1, the determination of the values associated to stream allocation and equipment sizing variables has been taken into account, while for the model presented in section 5.2 only the stream allocation-related ones had been determined (in order to ensure that the sizing-related variables are set as constant values throughout the analysed operational time set for the dynamic optimisation model). The two models overall considered the same set of assumptions and simplifications that have already been pointed for the optimisation model of case-study 1.

In Table 5-21, the comparison of the values associated to the main energy and water-use indicators obtained for all the phases of the exploitation of case-study (from the baseline case to the definitive optimisation configuration) are presented. In Figure 5.14, the flowsheet and stream allocation and sizing parameters values associated to the definitive optimised configuration are presented. The revised optimisation results in respect to specific system variables are presented in the sequence of Figures 5.15 – 5.18.

Table 5-21. Optimisation results for the main energy and water use indicators and its comparison with initial and previously obtained values (one cycle corresponds to 42 hours)

Utility/ Cost Parcel		Baseline Value	Scenario 2: With Electricity Production	Scenario 2: With Hydrogen Production	Optimised	Optimised (Effective)
Thermal Process System						
Natural Gas Flow Rate (kg/cycle)	Kiln 1	5355.00	4872.45	4872.45	4480.88	4530.38
	Kiln 2	5044.20	3992.10	3931.88	3456.20	3529.69
	Kiln 3	334.29	324.27	324.27	308.91	318.18
	Kiln 4	1266.05	1245.40	1245.40	1210.15	1230.65
Net Generated Electricity (kWh/cycle)			1437.81		470.47	771.89
Water System						
Freshwater Flow Rate (m^3/h)		0.861	0.419	0.460	0.529	0.529
Hot Utility Consumption (GJ/h)	Heater 1	0.125				
	Heater 2	0.180				
	Heater 3	0.033				
Cold Utility Consumption (GJ/h)	Cooler 1	0.085				
	Cooler 2	0.133				
	Cooler 3	0.017				
Overall						
Total Operational Cost (M€/year)		2.53	2.04	2.07	1.87	1.89

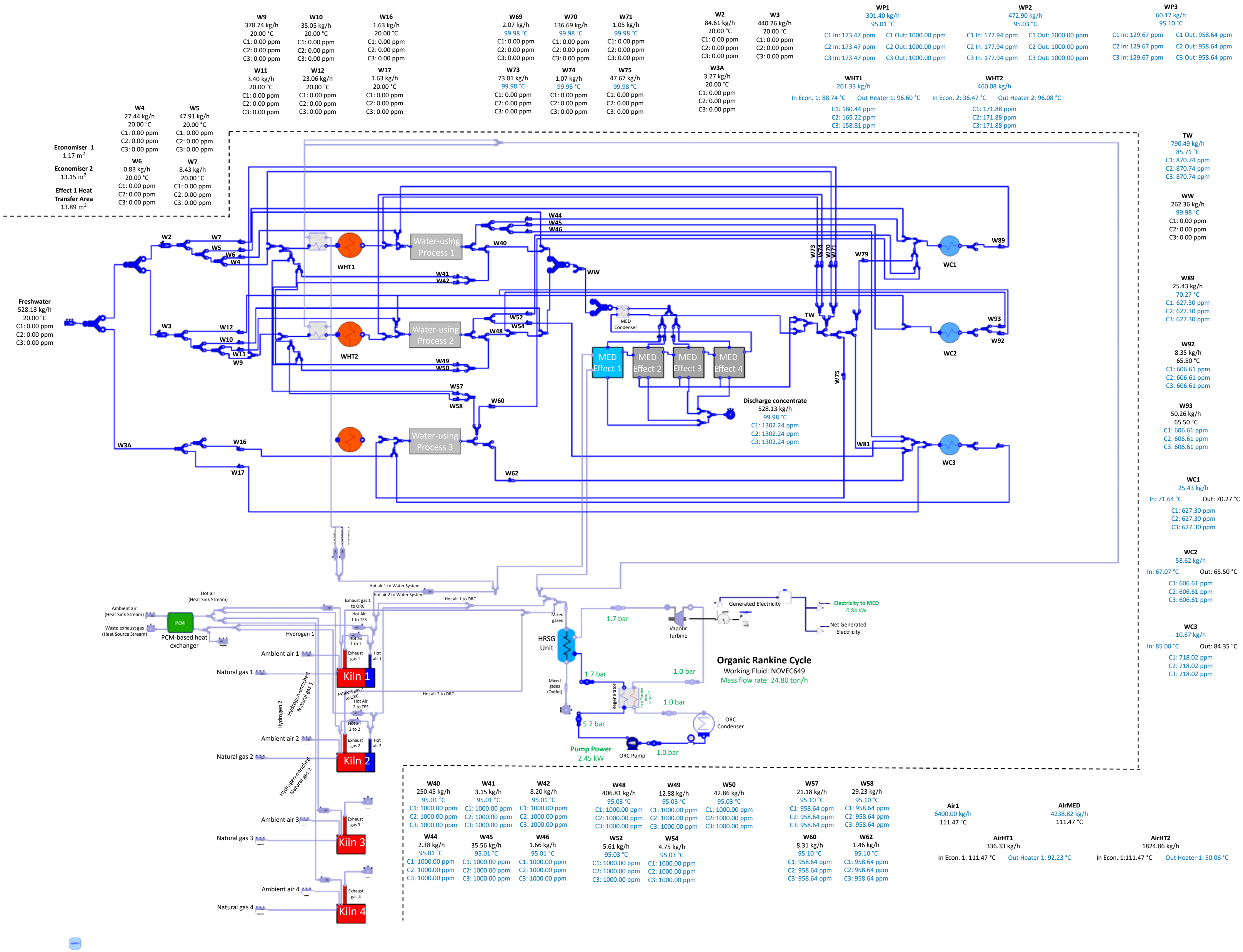


Figure 5.14. Flowsheet assembling of the Final Configuration for Case-study 2 WEIS model using the ThermWatt Modelica library capabilities (darker colour: corresponding values to the optimisation model, lighter colour: referent to variables that are only part of the simulation model)

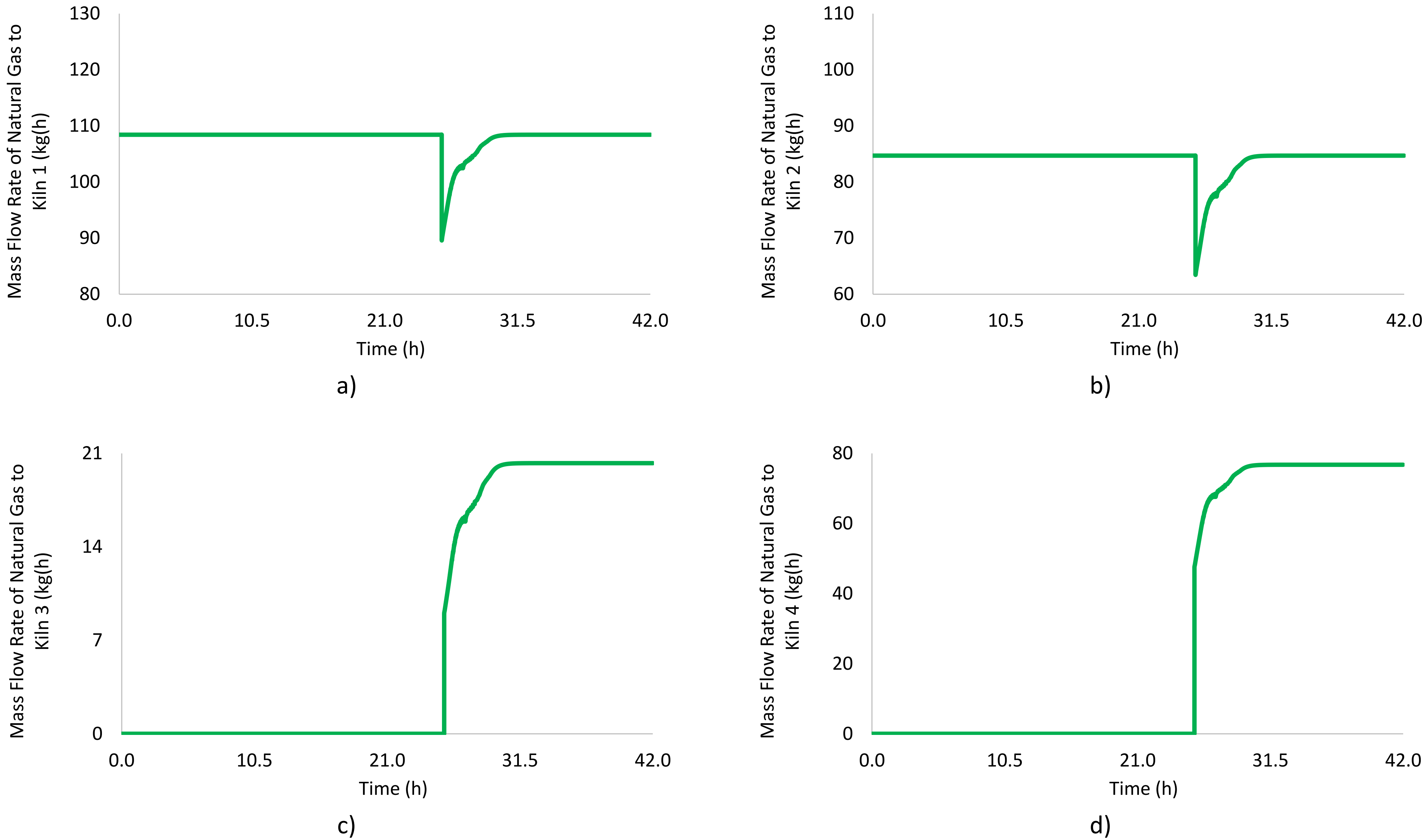


Figure 5.15. Final optimisation along time for the mass flow rate of natural gas of a) Kiln 1, b) Kiln 2, c) Kiln 3 and d) Kiln 4

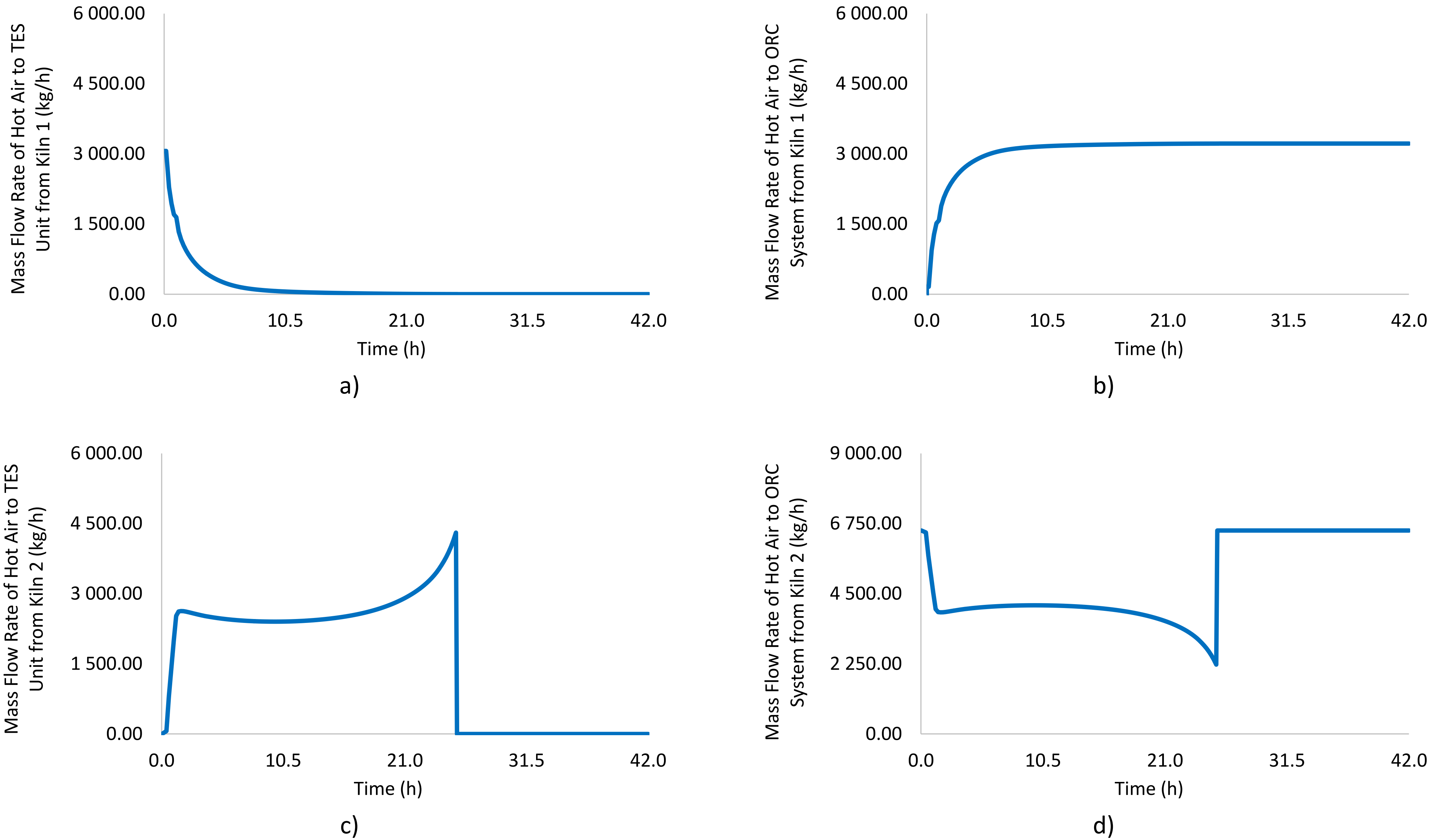


Figure 5.16. Final optimisation results along time for the mass flow rate of hot air form a) Kiln 1 to TES Unit, b) Kiln 1 to ORC System, c) Kiln 2 to TES Unit, d) Kiln 2 to ORC System

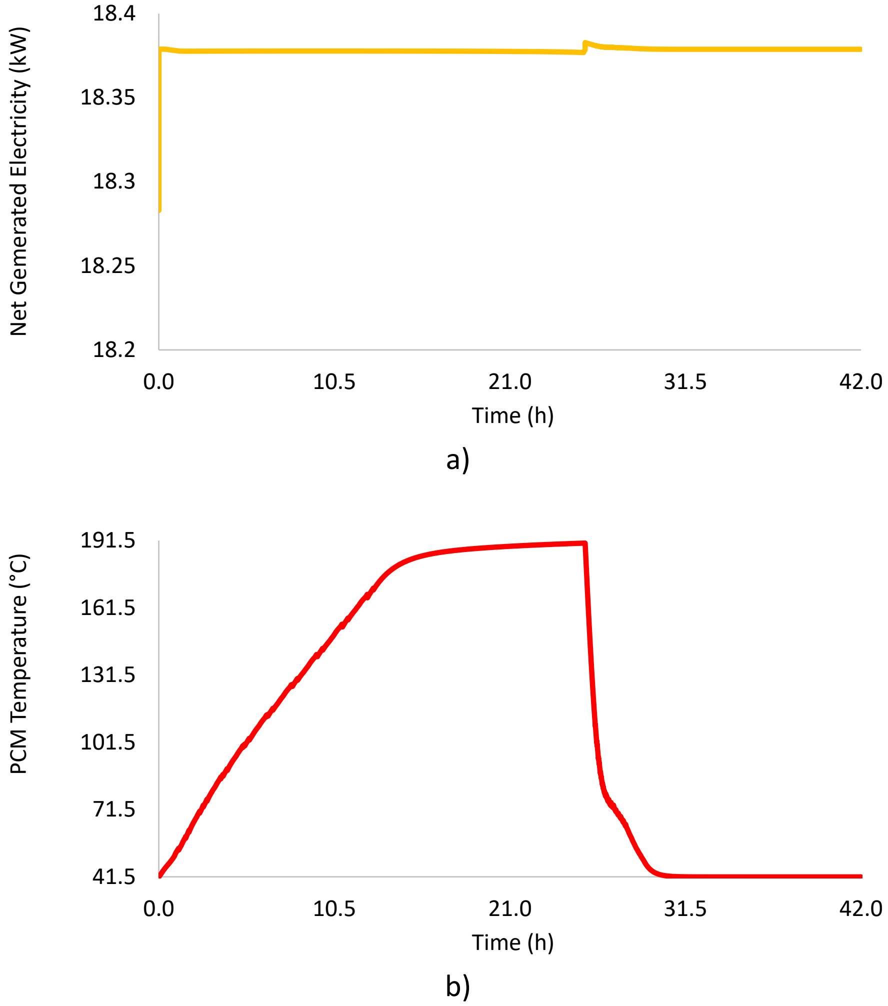


Figure 5.17. Final optimisation results along time for a) Generated electricity, b) Temperature of the PCM inside the PCM-based heat exchanger

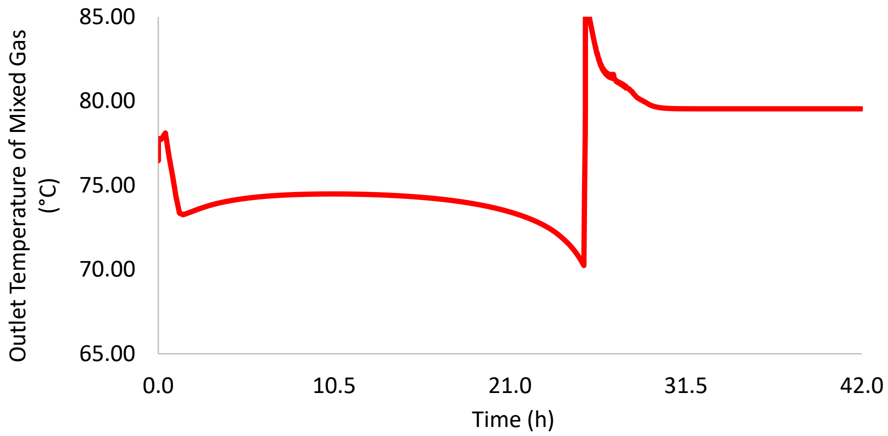


Figure 5.18. Final optimisation results along time for the temperature of the mixed gas at the outlet of the HRSG unit included in the ORC system

It is to note that while for the case of the water system optimisation model (NLP model) the exact same procedure related to the allocation of numerical results from case-study 1 was taken (the OpenModelica Python API incorporated into ThermWatt was used for the allocation of results from the Python model to the Modelica model), the thermal process system optimisation model uses a different procedure. In this case, a separate Modelica model script has been created, with an application programming interface (API) for the transfer of numerical values not being applied. The DP model developed for the thermal process system had necessarily to be developed in a separate layer which is not furtherly directly incorporated in the layer of the initially developed simulation model, owing to the incompatibility of the solvers used for the running of the two model counterparts (DASSL solver has been used for the simulation model, while for the DP model the internal solver designated as *optimization* has been used, with the latter being incompatible with the developed simulation model and the former not being set to be used for dynamic optimisation). An API similar to OpenModelica Python that allows the allocation of results between two Modelica models developed for different ends (in this case, dynamic optimisation and dynamic simulation) has still to be developed for the proposed objective of numerical result allocation.

The final flowsheet presented in Figure 5.14 shall be evaluated in terms of validity and optimal results. The standalone evaluation of validity shall be performed considering the two system parts that have been considered in the analysis of case-study 2: the water system and the thermal process system. For the water system, it may be observed an approximately exact correspondence of the values obtained for the counterpart variables. In respect to the thermal process system, it is possible to verify by the analysis of Figures 5.15 – 5.18 that the time-variating results obtained for the variables that have not been setup though defined values throughout time (in this case, natural gas flow rates and PCM temperature) present similar phases of variations, although not exactly corresponding due to different slopes associated to each variable variation with time. Such observation may be attributed to the simplifications performed for the modelling of heat transfer phenomena associated to the PCM-based heat exchanger in the thermal process system-associated DP model (which only considers two boundary conditions and one single node for the PCM temperature in the whole geometry of the heat exchanger). Based on the proposed objective of reducing total operational costs through thermal energy storage, it may be considered that the DP model has been at least able to produce on the final model the convergence to a point in which the storage of enthalpy is maximized (as may be verified by the achievement of the 191.5 ºC level for the PCM temperature which corresponds to the temperature of the hot air stream with the highest temperature) by not compromising simultaneous objectives (reduction of natural gas use and maximization of net generated electricity at each time instant).

In relation to the obtained profiles for net generated electricity and the outlet mixed gas temperature, it is possible to verify a lower variation of the generated electricity along with time (as may be observed through the comparison of Figure 5.12 – a) and Figure 5.17 – a)), with an inverted tendency being possible to be pointed out for the PCM temperature. Such may be explained due to the specific setup of the DP model developed for the thermal process system, namely in terms of the consideration of a constant value for the ORC thermal-to-electric conversion efficiency and the definition of the objective-function based on the maximization of net generated electricity (which allows for the convergence of the solution to a point in which the outlet mixed gas temperature reaches the lower bound of 70.0 ºC for all the instants of time). In the context of the final model, different operational conditions along with time cause a variation on the ORC thermal-to-electric efficiency, which is verified through an approximately constant level of net generated electricity across time for different values of withdrawn enthalpy (in its turn provoking different levels of the outlet mixed gas temperature).

Although it may be considered that the counterpart DP model has been successful in terms of optimal results related to the highest possible quantity of enthalpy stored in the conceptualized PCM-TES unit, further calibration procedures are necessary to allow a more consistent correspondence of results between models. Taking into account the observations pointed out for both system parts, it may be considered that the set of the two optimisation models and the final model are overall conceptually consistent. In this sense, the optimisation models have been capable to assess the optimal stream allocation-related values and the final model was able to assess the most effectively accurate values associated to those conditions.

In respect to optimised results, it may be mentioned that the net generated electricity is higher than the counterpart optimisation model owing to the purposed setup of the ORC thermal-to-electric to a considerably lower value than the one that is securely expected to be effectively obtained. In the context of the developed DP model, the assumption of a constant value for this variable may constitute a rough approximation at the light of the final results (obtained from a model that more accurately simulates the operation of the ORC system). However, at the light of the obtained results (in which the total natural gas use is minimized, stored enthalpy is maximized and net generated electricity is higher than the corresponding optimisation model results) such assumption may be considered pertinent.

Post-processing – Economic Evaluation and Environmental Impact Reduction Assessment

The computational models presented throughout chapters 4 and 5 have been developed with the ultimate aim to assist on the project of the installation of Water and Energy Integration Systems (WEIS), having the inherent capacity to estimate the values associated to all stream allocation and equipment sizing-related variables to systems which are set to promote overall eco-efficiency through recirculation. These have been primarily developed to minimize the input of energy and water in the system, while respecting the most basic constraints related to physical phenomena occurrence and operational constraints associated to plant maintenance. The project of the WEIS also required the project of the implementation of several technologies, which overall entail investment costs which are in all cases additional costs to the plant. These costs are overall related to the installation of the new machinery, maintenance of the installation and acquisition of new utilities.

The reduction of water and energy inputs in the water system is a guarantee that the environmental burden (resulting from the use of both these resources) is diminished in absolute values, as it is the case for the operational costs associated to these. With the aim to ensure that the project satisfies the requirements for it to be considered viable in respect to sustainability (economically and environmentally viable), it is necessary to proceed with both an economic evaluation and an environmental impact reduction assessment so to effectively ensure the simultaneous economic and environmental viability associated to the WEIS project. In Figures 5.19 and 5.20, the energy consumption levels for the whole plant for both the initial and improved scenarios associated to the main energy sources (natural gas, electricity and total final energy) are presented. In the sequence of Tables 5-22 and 5.23, it is presented the determination of the required indicators that lead to the effective economic evaluation and environmental impact reduction assessment of the previously presented WEIS projects for both case-studies 1 and 2. In respect to the performance of the presented assessments, the following assumptions and determination aspects are considered:

- The considered unitary water and energy prices are the ones that have already been used for the development of the optimisation models (23.66 €/GJ for natural gas, 0.1459 €/kWh for electricity and about 1.85 €/m^3 for freshwater), all summarized in appendix A9;
- The considered unitary equivalent carbon dioxide emissions factors are the ones covenanted for the energy system of Portugal [383] , all summarized in appendix A9;
- The investment costs associated to each asset of the WEIS project (from equipment to be installed to maintenance) are detailed in appendix A8. While the base cost for equipment has been determined according to formulas referred in equipment cost determination literature [260,384,385], the direct and indirect costs associated to the installation have been determined through the consideration of empirical factors for each direct and indirect cost parcel mentioned in Peters and Timmerhaus [386].

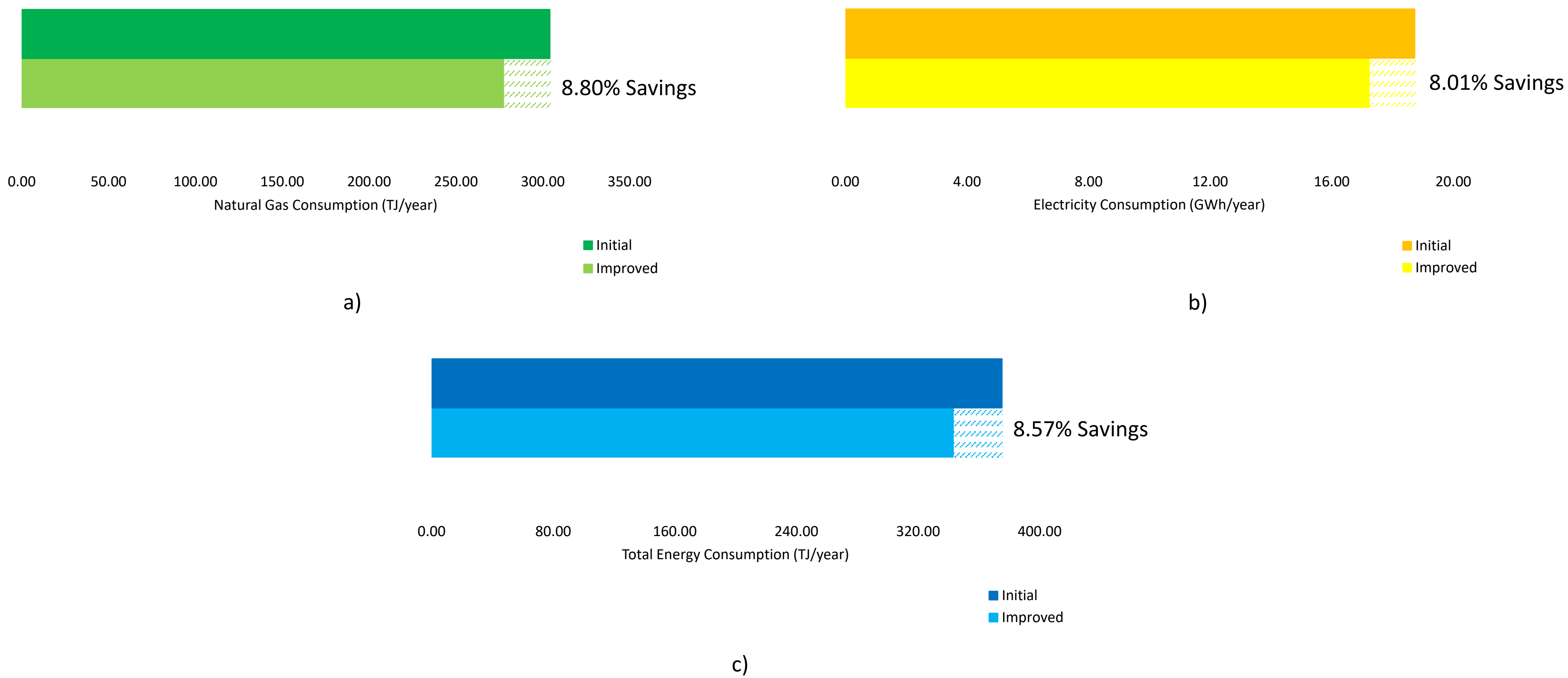


Figure 5.19. Comparison of consumption of energy sources between the initial and optimised cases for case-study 1, namely a) Natural Gas, b) Electricity, c) Total Energy

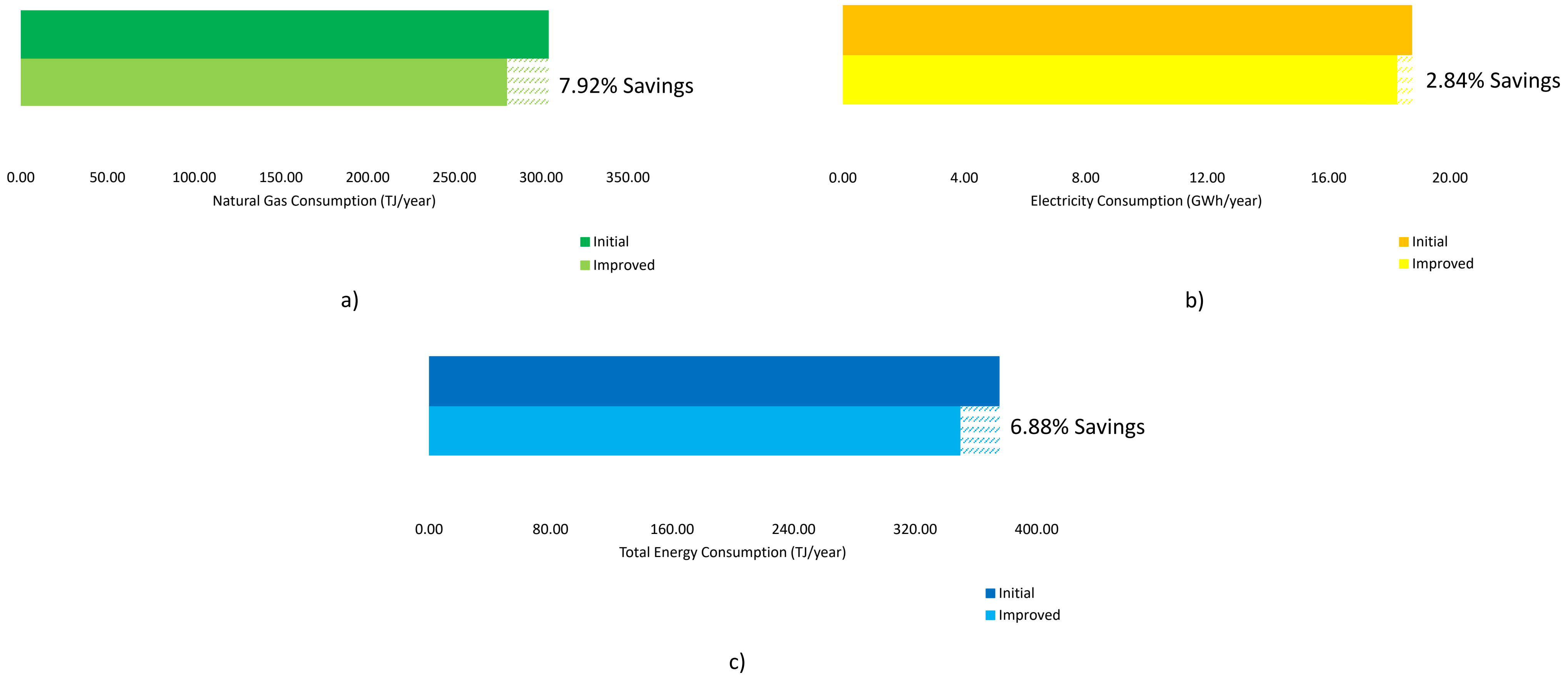


Figure 5.20. Comparison of consumption of energy sources between the initial and optimised cases for case-study 2, namely a) Natural Gas, b) Electricity, c) Total Energy

Table 5-22. Economic Evaluation and Environmental Impact Reduction Assessment for Case-study 1

Natural gas consumption (kg/h)				
Process	**Initial**	**Improved**	**Savings Share**	**Savings (€/h)**
Kiln 1	196.5	156.53	20.34%	42.65
Kiln 2	103.5	78.80	23.87%	26.36
Hot utilities consumption (GJ/h)				
Unit	**Initial**	**Improved**	**Savings Share**	**Savings (€/h)**
Heater 1	0.175	0.003	97.88%	4.05
Heater 2	0.183	0.003	97.83%	4.24
Heater 3	0.133	0.004	97.97%	3.08
Heater 4	0.023		100.00%	0.54
Cold utilities consumption (GJ/h)				
Unit	**Initial**	**Improved**	**Savings Share**	**Savings (€/h)**
Cooler	0.396		100.00%	16.05

Water consumption (m^3/h)			
Initial	**Improved**	**Relative Savings Share**	**Savings (€/h)**
1.378	1.051	23.71%	0.60

Electricity Balances (kWh/h)	
Net Electricity Generation (kWh/h)	**Savings (€/h)**
81.91	11.95

Final assessment		
Investment Cost (k€)	**Savings (k€/year)**	**Payback Time (Years)**
1538.32	856.94	1.80

Total $CO_{2,eq}$ Emissions Reduction (kton $CO_{2,eq}$/year)
2.42

Table 5-23. Economic Evaluation and Environmental Impact Reduction Assessment for Case-study 2

Natural gas consumption (kg/cycle)				
Process	**Initial**	**Improved**	**Relative Savings Share**	**Savings (€/cycle)**
Kiln 1	5355.00	4530.38	15.40%	879.92
Kiln 2	5044.20	3529.69	30.02%	1616.08
Kiln 3	334.29	318.18	4.82%	17.19
Kiln 4	1266.05	1230.65	2.80%	37.78
Hot utilities consumption (GJ/h)				
Unit	**Initial**	**Improved**	**Relative Savings Share**	**Savings (€/h)**
Heater 1	0.125		100.00%	2.958
Heater 2	0.180		100.00%	4.259
Heater 3	0.033		100.00%	0.781
Cold utilities consumption (GJ/h)				
Cooler 1	0.085		100.00%	3.439
Cooler 2	0.133		100.00%	5.374
Cooler 3	0.017		100.00%	0.689

Water consumption (m^3/h)			
Initial	**Improved**	**Relative Savings Share**	**Savings (€/h)**
0.861	0.529	38.57%	0.61

Electricity Balances (kWh/cycle)

Net Electricity Generation (kWh/cycle)		Savings (€/cycle)
771.89		112.62
Final assessment		
Investment Cost (k€)	**Savings (k€/year)**	**Payback Time (Years)**
1802.81	637.91	2.83
Total $CO_{2,eq}$ Emissions Reduction (kton $CO_{2,eq}$/year)		
1.76		

As may be verified though the analysis of Figures 5.19 and 5.20, the handling of the conceptualized Water and Energy Integration Systems (WEIS) projects considering the optimal scenarios for each case-study leads to significant savings at the level of each one of the approached energy sources. For both cases, the reduction of the total natural gas consumption is the most prominent benefit between all the energy-related benefits. Such may be attributed to the fact that both WEIS projects have been primarily conceptualized to reduce the fuel consumption in the combustion-based processes of each one of the analysed plants through the planning of heat recovery systems. Nonetheless, the reduction of electricity consumption is also considerable in both cases (although much more in case-study 1), and as such it may be mentioned that the project of the performance of heat recovery to produce additional electric energy through the installation of Organic Rankine cycle (ORC) systems in both cases is highly effective (considering that this electricity through the recirculation of streams that are otherwise considered as wastes).

In respect to the reduction of the freshwater consumption, it is possible to verify through the observation of the values obtained for the relative reduction in both case-studies (23.71% and 38.57% for case-studies 1 and 2, respectively) that the projected water recirculation network is effective not only in the aspect of generating savings in the total consumption of hot and cold utilities but also for the considerable improvement of water efficiency. The relative reduction levels obtained for the approached water systems are comparable to a 18% water saving potential estimated for a model industrial park [387].

The assessment of both WEIS projects converges on the determination of the economic and environmental viability associated to these. In the context of the present analysis, such determination has as a basis the analysis of the payback period and the absolute $CO_{2,eq}$ emissions reduction respectively, which have been obtained taking into account the optimal configurations obtained for each case-study. In relation to the estimated payback period values (about 22 months for case-study 1 and 34 months for case-study 2), two benchmarks values may be used: a 2 – 3 years (24 – 36 months) reasonable payback period interval for energy efficiency improvement measures within the industry of the European Union [388] and a 5 years (60 months) limit for a technology to be considered viable for industry in general [389]. For both case-studies 1 and 2, it is possible to verify that the obtained payback period is considerably lesser than the first mentioned benchmark interval. In this prospect, it is possible to affirm that the WEIS projects of both case-studies are securely favourable in comparison to the strictest benchmark (24 – 36 months).

The determination of the environmental impact reduction-associated viability for both installations depends in its turn on the comparison of the estimated reductions of $CO_{2,eq}$ emissions on benchmark values obtained for the approached industrial sector (in this case the European Union ceramic industry). Considering the obtained values (2.42 and 1.76 kton $CO_{2,eq}$/year, respectively for case-studies 1 and 2) and taking into account different values for energy efficiency improvement measures implementation within the analysed sector (corresponding to a maximum value of 0.722 kton $CO_{2,eq}$/year [390]), it may be considered that the conceptualized WEIS project is effective in terms of the reduction of the environmental impact brought by the operation of the plant-level energy systems. The total ecological footprint reduction potential associated to the project is enforced by the zero-water discharge level obtained for each one of the case-studies, in which the only discharged streams of the water systems correspond to the brine streams from wastewater treatment (in this case the Multi-effect distillation units).

In respect to the generation of the brine streams in the context of the projected desalination units, it is to note that the conceptualized WEIS installations have been approaching the achievement of the objective associated to water and energy recirculation and respective benefits, not being extended to the issues related to the generated brine disposal. Nonetheless, it may be mentioned that the total environmental impact associated to the operation of the plant may be reduced through the implementation of the detailed projects, since the total salt quantity at the downstream of the water systems is at least equal for both case-studies. Furthermore, since the commissioning of WEIS in real-life plants is accompanied by the installation of several piping sections, as well as a complex control and monitoring system, the planning of brine discharges is facilitated, which furtherly facilitates brine recovery (as either nutrients in soils or to-be-valorised energy).

6. Sustainability and Strategic Assessment

The integration between simulation and optimisation models developed in the previous chapters led to the achievement of substantial improvements at the level of the energy and water use within the approached case-study plants, through the determination of the point of the projected Water and Energy Integration Systems (WEIS) which is considered to be optimal. The whole procedure including model development, WEIS conceptualization and process and energy system optimisation converged on the achievement of the primary aims of this work related to the proof of the concept of WEIS, the development of an innovative computational tool to implement such concept and the obtainment of results related to the essential benefits categories of energy efficiency improvement, water efficiency improvement and pollutant emissions reduction. A post-processing assessment based on the determination of economic and environmental impact reduction viabilities for the selected installations was furtherly performed.

At the light of the determination of the sustainable character associated to the proposed projects, the latter assessments led to the ascertainment of the viability of the referred projects in a primary form, namely through the comparison of the payback period and estimated equivalent carbon dioxide emissions for defined benchmarks. The economic and environmental viability character assessed for the conceptualized WEIS shall be reinforced through the determination of several indicators which translate the promotion of both the eco-efficiency and circular economy characters associated to the conceptualized installations. Furthermore, with the objective to effectively and fully prove the sustainability promotion potential associated to these installations, the obtained benefits shall be compared with the strategic objectives defined in the most recent energy and water use-related policies in the world, which in its turn are in line with the requirements inherent to promotion of economic savings end environmental impact reduction in the context of social benefits.

In this chapter, it is performed an assessment of several eco-efficiency and circular economy character promotion indicators for the conceptualized installations, as well as an assessment of the effective fulfilment of the estimated benefits in terms of strategic objectives. In general, such integrated assessment shall prove and reinforce the sustainability promotion character associated to the concept of Water and Energy Integration Systems, in particular the proper case-studies projected systems.

A set of publications have been developed by the authors in which the described methodology is implemented for the approached case-studies and another industrial sector [391,392].

General Framework

This chapter aims to perform a verification of the inherent capacity of the conceptualized Water and Energy Integration Systems to be sustainable. In this prospect, it is performed an integrated assessment divided in two parts:

- One in which several eco-efficiency and circular economy character promotion indicators (related to the optimised scenarios of the case-studies) are determined;
- A second in which it is performed an analysis on the strategic aims delineated in the most recent sustainability policies and ones related to mitigation of the most recent social issues. These aims are compared to the case-studies results based on specific numerical indicators considered in these policies and for the purpose of measuring the impacts of the aforementioned social issues.

The overall verification of the correspondent case-study results with the promotion of eco-efficiency and circular economy character and the aforementioned strategic aims is considered to be a necessary and sufficient condition to prove the sustainability character of the conceptualized installations, taking into account the three dimensions of the sustainability concept. In Figure 6.1, the described rationale is pictorially presented.

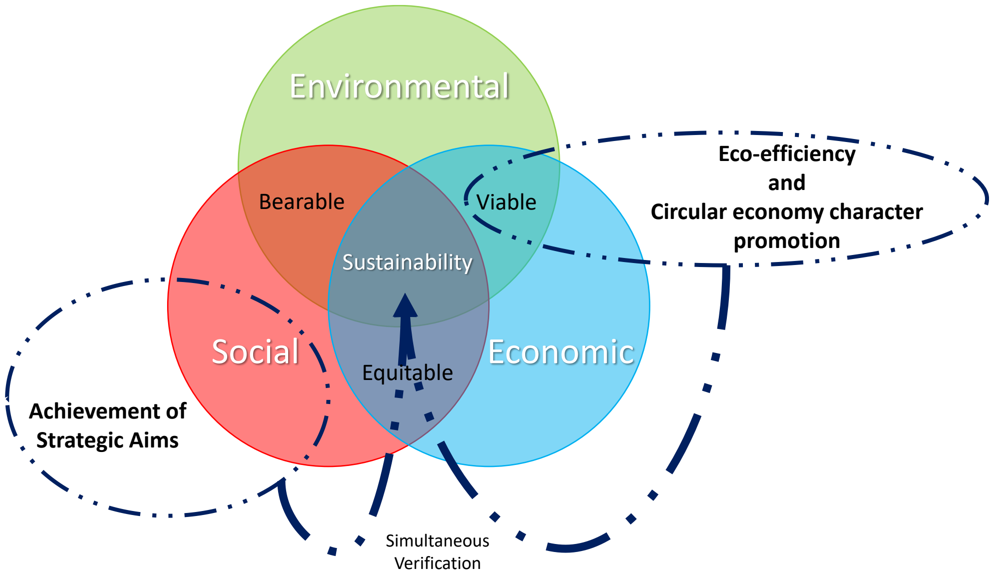


Figure 6.1. Context of the general objectives of the work within the three dimensions of Sustainability

At the light of the concept presented in Figure 6.1, the economic and environmental viability associated to conceptualized Water and Energy Integration Systems (WEIS) is set to be reinforced (in comparison to previously obtained results from the economic evaluation and environmental impact reduction assessment performed to case-studies) by the determination of eco-efficiency and circular economy character promotion indicators (as it is set to be proceeded in section 6.1). On the other hand, the promotion of the social aspect (as it is set to be proceeded in section 6.2) associated to the installations (potential associated to the mitigation of social impacts) is set to be assessed through the determination of specific indicators to be compared with the specific aims pointed out in the most recent sustainability policies, as well as the specific indicators expressing the impacts of the most recent social issues. It is intended that with the adequacy of the results obtained in the context of the case-studies with the specific aims that the promotion of social stability-related aspects pointed out in the most recent policies is also secured, being assumed a direct correlation between the verification of the compliance with the approached strategic aims with the social-related (that are not directly assessed).

6.1. Assessment of Eco-efficiency and Circular economy character promotion Indicators

The final results obtained for the selected case-study plants may be interpreted at the light of the indicators that measure the economic and environmental viability associated to the installations. Such analysis must be performed bearing in mind that the improved scenario for a plant (which in this case is defined as the optimal scenario obtained by the performance of the optimisation procedures) must be associated to improved levels of each defined indicator.

In the scope of the present analysis, the indicators that are set to be determined are of the following categories:

- Eco-efficiency promotion (indicators that express the potentially improved economic value to environmental burden ratio);
- Circular economy promotion (indicators that express the capacity of the projects for the performance of recycling and reuse).

The determination methods for each one of the eco-efficiency and circular economy character promotion indicators have been characterized in section 3.5.

6.1.1. Determination and Analysis of Eco-efficiency promotion Indicators

The assessment of eco-efficiency promotion with the analysed installations may be performed by the analysis of indicators that either express the increase of the economic value associated to the project or the decrease of the environmental burden (or the conjugation of both). The effective analysis of the improved eco-efficiency of the analysed installations must be performed by the integrated analysis of all the proposed indicators, rather on the analysis of single indicators that express achieved benefits in terms of only one of the dimensions of sustainability. Such procedure is performed to ensure that eco-efficiency promotion win respect to the proposed projects is effective. In Tables 6-1 and 6-2, proposed indicators for the eco-efficiency promotion characterization determined for case-studies 1 and 2 are respectively presented. For the propose of further analysis, the determination of indicators is performed for both the baseline and improved scenarios. In respect to the improved scenarios, two sets of results are defined for monetary-based indicators:

- One designated as Beginning-of-life corresponding to a scenario at the point in time of the acquisition of the required technology and machinery for the commissioning of the WEIS (in which the total investment cost is considered as a negative parcel for the determination of the improved scenario revenue);

- Another designated as End-of-life corresponding to a scenario in the immediate point in time following the return on investment (in which the total investment cost is not already considered as a parcel).

The values obtained for the aforementioned sub-scenarios thus constitute minimum and maximum values possible to be obtained for the indicators in question.

Table 6-1. Determination of Eco-efficiency indicators relative to Case-study 1

Indicator	Baseline Scenario	Improved Scenario	
		Beginning-of-life	End-of-life
Energy use-related indicators			
Specific Natural Gas Consumption (GJ/ton)	8.58	7.83	
Specific Electricity Consumption (MWh/ton)	0.53	0.49	
Water system-related indicators			
Specific Water Consumption (m^3/ton)	0.30	0.23	
Water energy footprint (MJ/m^3)	660.38	9.88	
GHG emissions-related indicators			
Produced material emission intensity (ton $CO_{2,eq}$/ ton material)	0.81	0.74	
Energy carbon footprint (ton $CO_{2,eq}$/ TJ)	76.11	76.19	
Aggregated Eco-efficiency indicators			
Aggregated Eco-efficiency indicator (€/kg $CO_{2,eq}$)	0.75	0.75	0.80 (6.46% promotion)
Produced material productivity (€/kg material)	0.93	1.02	1.08

Table 6-2. Determination of Eco-efficiency indicators relative to Case-study 2

Indicator	Baseline Scenario	Improved Scenario	
		Beginning-of-Life	End-of-Life
Energy use-related indicators			
Specific Natural Gas Consumption (GJ/ton)	8.58	7.90	
Specific Electricity Consumption (MWh/ton)	0.53	0.51	
Water system-related indicators			
Specific Water Consumption (m^3/ton)	0.19	0.12	
Water energy footprint (MJ/m^3)	665.85	1.01	
GHG emissions-related indicators			
Produced material emission intensity (ton $CO_{2,eq}$/ ton material)	0.81	0.76	
Energy carbon footprint (ton $CO_{2,eq}$/ TJ)	76.11	76.72	
Aggregated Eco-efficiency indicators			
Aggregated Eco-efficiency indicator (€/kg $CO_{2,eq}$)	0.75	0.73	0.78 (4.00% promotion)

Produced material productivity (€/kg material)	0.93	0.97	1.04

The analysis of the results for the indicators determination presented in Tables 6-1 and 6-2 will be performed by analysing each one of the categories in which the mentioned indicators were divided:

- The energy use-related indicators are formulated to express the energy consumption in relation to total material production (which is set as the same value for both the baseline and improved scenarios), thus subsisting on a measure of the productivity of the plant in relation to energy costs;
- The water system-related indicators are formulated to express water use in relation to total material production and the energy dependence of the water system;
- The GHG emissions-related indicators shall express not only the environmental footprint but also the level of pollutant emissions against the total use of one of the resources in question (for instance, the level of total GHG emissions in relation to the total energy consumption);
- The aggregated eco-efficiency indicators shall subsist on the relation between the total achieved benefits in terms of increased economic value (achieved through the reduction of energy and water costs) and the reduced environmental burden (achieved through the reduction of pollutant emissions).

The results obtained for the proposed indicators for case-study overall express the effective promotion of eco-efficiency achieved by the implementation of the WEIS project. In Table 6-3, it is presented the interpretation of the obtained results for the approached indicators.

Table 6-3. Interpretation of results obtained for eco-efficiency promotion indicators

Category	Interpretation
Energy use-related	• It is possible to verify that a considerable decrease may be achieved by the implementation of the proposed project, with this reduction being significant in the case of natural gas use; • In comparison to benchmark values obtained for European industry, the achieved levels of specific energy consumption are still above the average levels obtained for selected ceramic industry companies (6.09 GJ/ton in comparison to the obtained 7.76 GJ/ton and 7.98 GJ/ton for case-study 1 and case-study 2 natural gas, respectively, and 0.19 MWh/ton in comparison to the obtained 0.49 MWh/ton and 0.51 MWh/ton for electricity, respectively [393]); • Nonetheless, it may be affirmed that the project is effective for the approximation of the energy use levels to the average of European industry, with such effective approximation being potentially achieved through the implementation of complementary energy efficiency improvement measures to the ones considered in the project of the WEIS.
Water system-related	• It is possible to verify relative improvements for both the analysed indicators between the baseline and improved scenarios of case-studies 1 and 2; • In comparison to benchmark values obtained for European industry, the obtained levels of specific water consumption are comparable to the ones obtained for both the wet and dry routes of ceramic tile production (0.47 – 0.59 m^3/ton and 0.12 – 0.16 m^3/ton, respectively [394]), although the potential associated to the water recirculation procedure associated to the conceptualized system falls short in comparison to the substitution from wet to dry routes in the referred sub-sector of the ceramic industry (which is associated to about 74% water savings);

	• In relation to the Water energy footprint, the relative decrease between the baseline and improved scenarios for both case-studies is significant of a decrease of the energy dependence of the water system, in which a lesser total energy input is required for the operation of the water system considering the respective freshwater consumption levels. At the light of these results, it is possible to affirm that the conjoined performance of water recirculation and hot air recirculation to the enthalpy-using units within the water system (in this case, economisers and the MED unit) generates an operational point in which the self-sufficiency of the water system in terms of enthalpy allocation increases.
GHG emissions-related	• In relation to the produced material GHG emissions intensity, it is possible to verify considerable improvements for both case-studies. Nevertheless, the emission intensity estimated for the improved scenarios are still higher than benchmark values (0.329, 0.338 and 0.263 (in two different plants) ton $CO_{2,eq}$/ ton material for the production of four different tile products, respectively [390]); • In relation to the energy carbon footprint indicator, it is possible to verify an increase between the baseline and improved scenarios for both case-studies 1 and 2. Such increase may be interpreted at the light of the relative decreases of the use of each of the energy sources in questions and the emission factor associated to each energy source: the relative decrease of natural gas consumption is higher for both cases than the electric energy consumption, although the tabled emission factor for natural gas is lower than the one for electricity (64.1 kg $CO_{2,eq}$ /GJ and 0.47 kg $CO_{2,eq}$ /kWh corresponding to 130.56 kg $CO_{2,eq}$/GJ, respectively). As such, the highest relative decrease of natural gas consumption allows for the representativity of the electric energy consumption of the plant in the improved scenario to be higher, thus augmenting the ratio between the total $CO_{2,eq}$ emissions and total energy consumption. At the light of the implementation of the WEIS project, such increase is not significant for the evaluation of the project in terms of economic and environmental viability, just being indicative of the dislocation of the energy efficiency improvement project towards natural gas reduction.
Aggregated Eco-efficiency	• It is possible to verify improvements between the baseline and the end-of-life improved scenarios for both case-studies for the two approached indicators; • The pointed increase of the aggregated eco-efficiency indicator may be attributed to both an increase of the economic value associated to the plant and the decrease of the energy use-related environmental burden; • The increase of material productivity is indicative that the generated economic savings through the implementation of the WEIS increases the economic value of production for the same level of produced ceramic material; • For case-study 2, it is possible to verify that the aggregated eco-efficiency indicator is lower for the improved scenario in the defined beginning-of-life stage, which may be interpreted as the capacity of the conceptualized WEIS to create economic value in relation to the energy-use related environmental burden only in a determinate point of the project lifetime.

Taking into account the verifications detailed in Table 6-3, it is possible to affirm that the for both the approached case-studies it exists a reasonable level of eco-efficiency promotion related to the economic and environmental burden reduction benefits generated by the decrease of energy and water-related costs. Nevertheless, it has been identified that the WEIS project shall be accompanied by the implementation of further measures, in particular energy efficiency improvement ones, with the aim to contend with benchmark values pointed for the approached industrial sector.

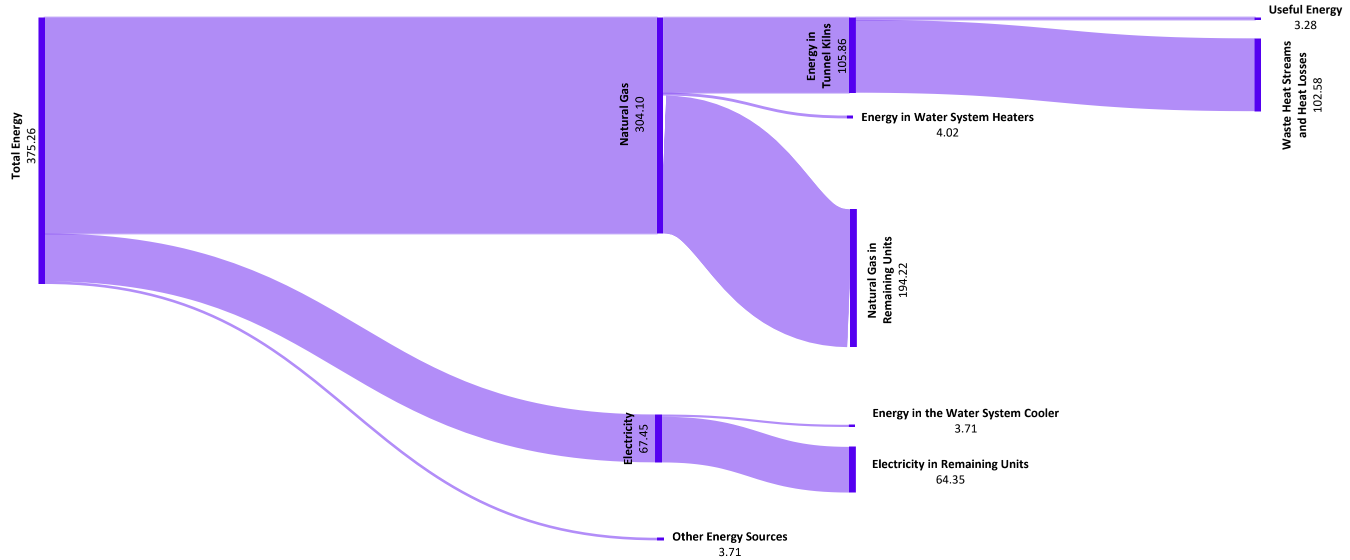
6.1.2. Determination and Analysis of Circular Economy character Indicators

The potential for the promotion of the circular economy character associated to the project of Water and Energy Integration Systems (WEIS) is derived from the inherent attribute of these being essentially closed-loop systems (or rather systems with reduced input and output of energy and water-related streams in comparison to open-loop ones). The project of WEIS is based on the promotion of practices such as recycling, reuse and by-pass of to-be-valorised energy and water streams. These phenomena (which are pillars of the concept of circular economy) have been conjointly referred in this work as recirculation.

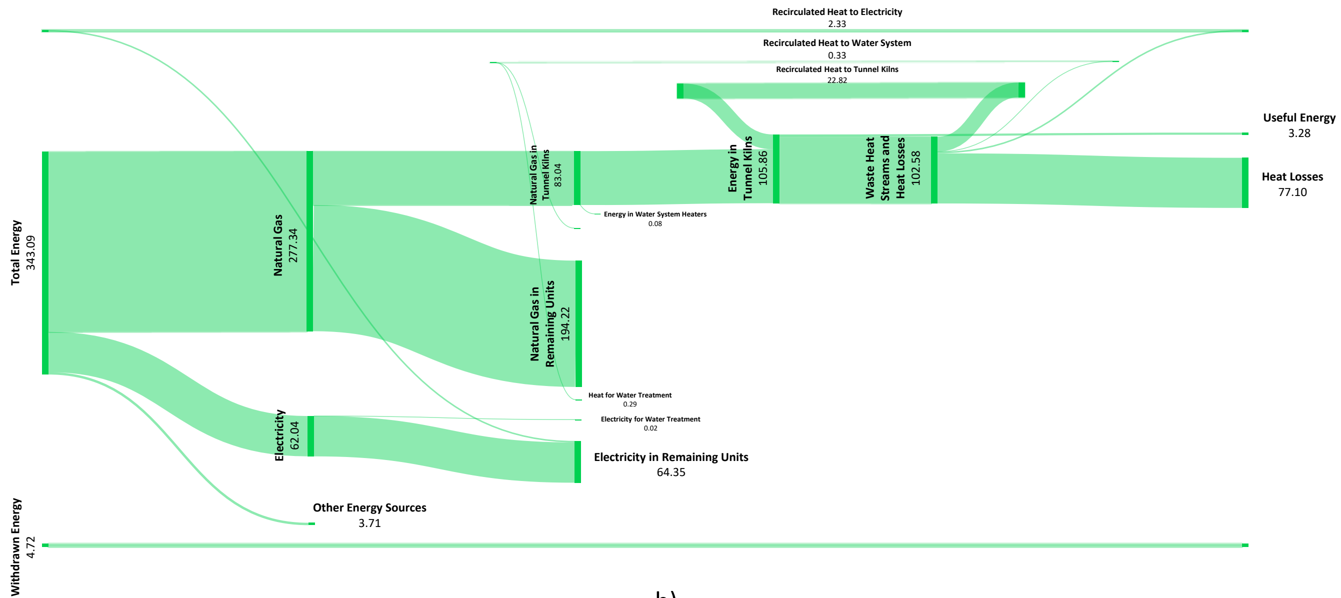
The distinction between standard energy and water efficiency improvement measures and WEIS implementation resides on the characteristic of the latter for using recirculation for the achievement of purposes related to decarbonisation, and in a further step eco-efficiency. In this prospect, the conceptual aim of the WEIS may be enunciated as the promotion of both low-carbon and circular economies in an optimised manner bearing in mind the objective of the maximization of eco-efficiency.

In a social perspective, the concept of circular economy has been facing critiques in terms of it being vague and metaphorical in nature [395]. It is to note that objective of this work is not the achievement of the proof of such concept, only gather elements from it and implement these within an innovative concept. Nonetheless, it is of relevance the establishment of the relation between the findings obtained for the study of WEIS to the specific features of the circular economy concept, so to furtherly establish a relation to the aims of the most recent sustainability policies.

The circular economy character associated to the conceptualized WEIS is set to be assessed in this work primarily through the development of diagrams that detail the energy fluxes in the plants, namely through the flux from the total energy consumption in a plant (corresponding to the final energy receive by the plant) to the useful energy and energy losses (in this case, the energy losses parcels of interest are the ones corresponding to waste heat streams). A set of indicators is also set to be determined. Since water consumption within the analysed case-studies are not associated to such a complex division of different uses, the circular economy character associated to this resource is enforced by the determination of several indicators. In Figures 6.2 and 6.3, the Sankey diagrams that details the energy fluxes for the baseline and improved scenarios for case-studies 1 and 2 are respectively presented. The determined values associated to circular economy-related potential indicators for case-study 1 and 2 are respectively presented in Tables 6-4 and 6.5.

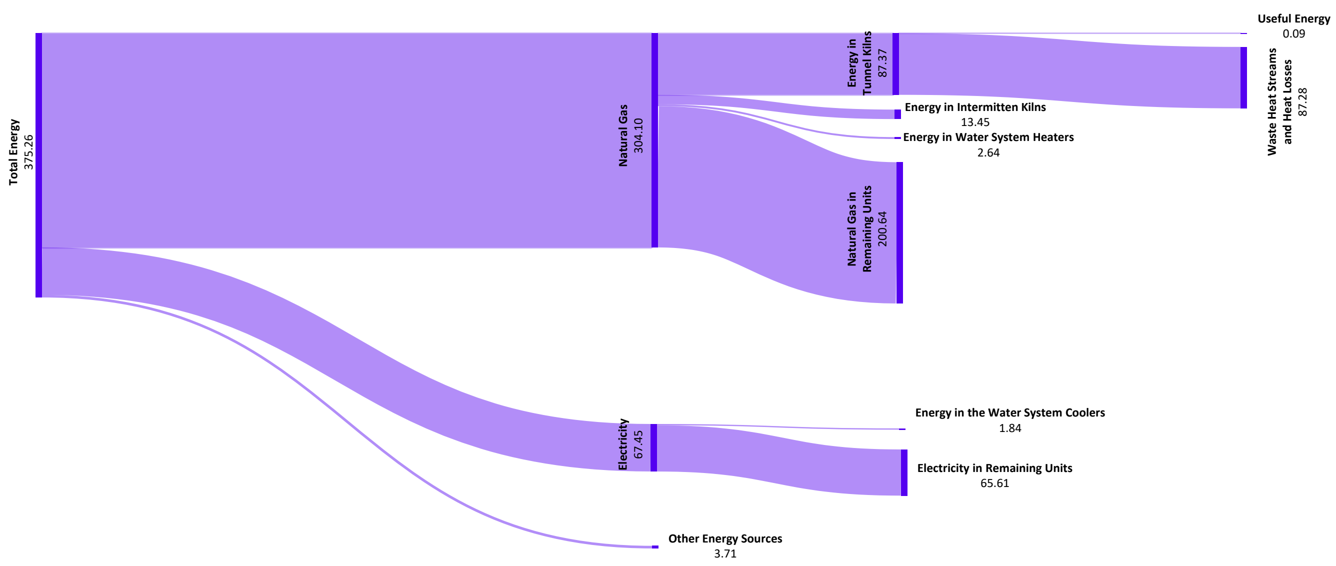


a)

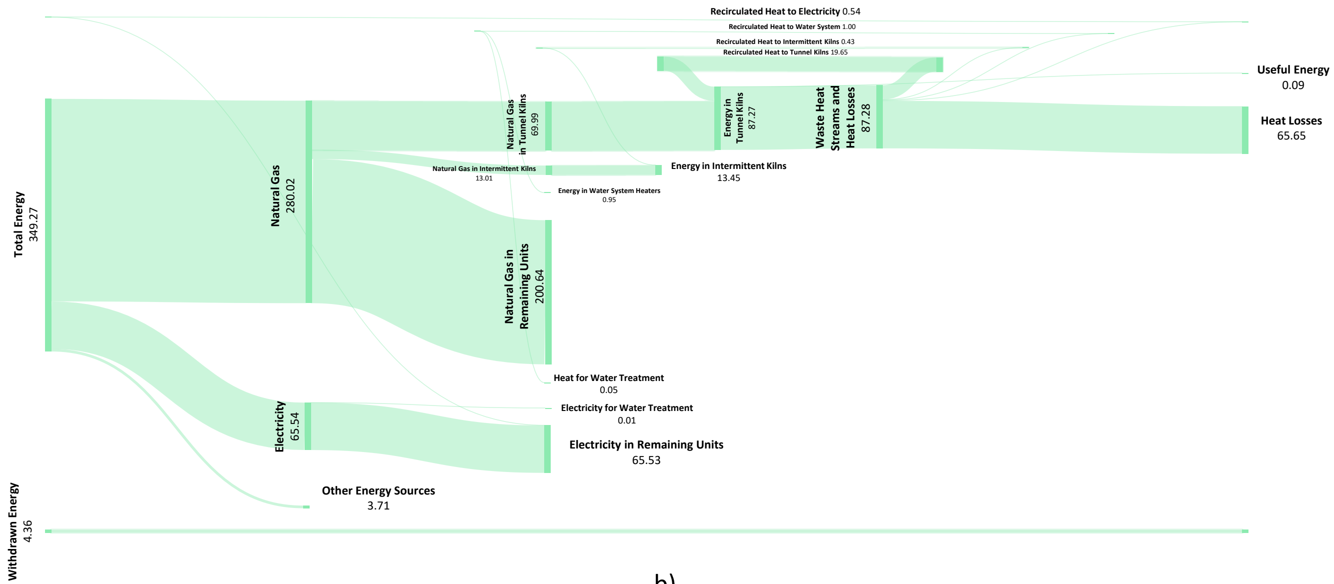


b)

Figure 6.2. Sankey Diagram for the Plant Energy Balance in Case-study 1: a) Baseline Scenario, b) Improved Scenario (Energy consumption unit of TJ/year)



a)



b)

Figure 6.3. Sankey Diagram for the Plant Energy Balance in Case-study 2: a) Baseline Scenario, b) Improved Scenario (Energy consumption unit of TJ/year)

Table 6-4. Determination of Circular economy promotion-related indicators relative for Case-study 1

Indicator	Baseline Scenario	Improved Scenario
Energy use-related indicators		
Waste Heat to Total Energy Ratio	27.34%	23.25%
Recirculated Heat to Baseline Total Energy Ratio		8.58%
Waste Heat to Natural Gas Used in Combustion-based Processes Ratio	96.90%	96.05%
Recirculated Heat to Baseline Natural Gas Used in Combustion-based Processes Ratio		38.76%
Water use-related indicators		
Discharge Water to Freshwater Ratio	100.00%	0.00%
Treated water to Wastewater Ratio		24.25%
Recirculated to Produced Treated Water Ratio		100.00%
Recirculated Treated Water to Water Savings		103.14%
Energy Input in the Water System-related Indicators		
Energy in Water System in the Improved Scenario over the Baseline Scenario		34.15%
Withdrawn Energy from the Water System in the Improved Scenario over Energy in the Water System in the Baseline Scenario		66.36%

Table 6-5. Determination of Circular economy promotion-related indicators relative for Case-study 2

Indicator	Baseline Scenario	Improved Scenario
Energy use-related indicators		
Waste Heat to Total Energy Ratio	23.26%	19.71%
Recirculated Heat to Baseline Total Energy Ratio		6.69%
Waste Heat to Natural Gas Used in Combustion-based Processes Ratio	46.38%	45.55%
Recirculated Heat to Baseline Natural Gas Used in Combustion-based Processes Ratio		16.91%
Water use-related indicators		
Discharge Water to Freshwater Ratio	100.00%	0.00%
Treated water to Wastewater Ratio		33.19%
Recirculated to Produced Treated Water Ratio		99.21%
Recirculated Treated Water to Water Savings		78.50%
Energy Input in the Water System-related Indicators		
Energy in Water System in the Improved Scenario over the Baseline Scenario		22.82%
Withdrawn Energy from the Water System in the Improved Scenario over Energy in the Water System in the Baseline Scenario		77.29%

The assessment of the circular economy character for the conceptualized installations encompassed by the results presented in Figures 6.2 and 6.3 may be conceptually performed either on basis of the comparison to the total resource comparison of the generated waste streams (waste heat and discharge water) or the recirculated streams. The indicators selected to be calculated and furtherly presented in Tables 6-4 – 6-5 are generally of both categories, and such option of determination was selected so to proceed with circular economy-related potential based on both benefits achieved by the implementation of closed-loop systems (recirculation promotion and waste reduction). In Table 6-6, it is presented the interpretation of the afore presented results at the light of the implication of these on circular economy promotion.

Table 6-6. Interpretation of results obtained for the circular economy-related potential promotion

Category	Interpretation
Energy use-related	• It is possible to observe that for both waste reduction-type indicators (Waste Heat to Total Energy Ratio and Recirculated Heat to Natural Gas Used in Combustion-based Processes Ratios) a considerable reduction occurs between the baseline and improved scenarios correspondent to case-studies 1 and 2. Such verification may be attributed to a superior capacity of the conceptualized WEIS to favour the reduction of the output of the energy-using units (waste heat) over the energy input (total energy and natural gas); • The recirculation promotion-based indicators (Recirculated Heat to Baseline Total Energy and Recirculated Heat to Baseline Natural Gas Used in Combustion-based Processes) in its turn shall give a measurement of the effectiveness of recirculated waste heat streams for the fulfilment of the energy requirements of the plants. As may be verified by the analysis of the sequence of Figures 6.2 and 6.3 and Tables 6-4 – 6-5, the recirculated heat streams correspond to a considerable part of the total energy and natural gas supply levels of to the baseline scenario (which correspond to total energy requirements, either through energy input or energy recirculation), thus proving the effectiveness of waste heat recovery within the conceptualized system. Nonetheless, the total energy input (non-recirculated energy parcels) is still the most representative; • Considering that the existing to-be-valorised heat streams in the plants have been recirculated to the maximum point of valorisation (in which the whole enthalpy that is possible to be recovered have been withdrawn from these streams), the verifications pointed for both indicator categories reinforce the aforementioned identified need to furtherly implement alternative energy efficiency improvement measures within the industrial processes existing in the plant, so to effectively reduce the energy inputs.
Water use-related	• It is possible to verify through the analysis of the sequence of values obtained for the approached indicators that water recirculation within the conceptualized water system has been extensively promoted; • For both cases, the ratio of discharge water to the inlet freshwater is null, due to the null discharge water (the only outlet streams from the water systems is the concentrate streams from the MED units); • The values obtained for the ratio between produced desalinated water and inlet saline water in the MED units of both case-studies are relatively low in comparison to the water savings requirements of the conceptualized system. Such indicator may be eventually improved through the installation of a high number of effects for the MED unit, in its turn promoting both water and enthalpy recirculation within the water system; • The recirculated to produced treated water ratio obtained for both case-studies is relatively high, being 100% for case-study 1 (which is akin to affirm that all the produced desalinated

	water is effectively recirculated). It is to note that the assessment of such indicator is relevant so to evaluate that the recirculation of treated water is not affected by another requirement, such as hot and cold utility minimization and the other recirculated streams within the water system which may be considered secondary (as treated water shall be desirably recirculated owing to its extensively minimized salt concentration). Although treated water recirculation is not affected by remaining requirements in case-study 1, for case-study 2 these requirements are preponderant, leading to the convergence of the developed optimisation model to a point in which a part of the total treated water quantity remains on the main water-using line. • The values obtained for recirculated treated water to water savings ration denotes are significantly high, denoting that the recirculation of treated water is mostly significant for the production of water savings, although the recirculation of secondary water streams has still a considerable contribution in such savings.
Energy Input in the Water System-related	• The **Energy in Water System in the Improved Scenario over the Baseline Scenario** indicator serves to assess the energy input related to the improved scenario (encompassing the input of hot and cold utilities proper, the enthalpy allocated from hot air to the economisers and to the MED unit) in relation to the hot and cold utilities input in the baseline scenarios. Such comparison allows to assess the potential of the valorisation of the recirculated streams to cause energy savings rather than to fulfil additional energy requirements (such as the ones related to wastewater treatment). For both case-study 1 and 2, such indicator is considerably low, which is significant of a total energy dependence of the water system (to both hot and cold utilities and recirculated heat from combustion-based processes) owing to water stream recirculation; • The previous affirmation is supported by the significantly high value obtained for the **Withdrawn Energy from the Water System in the Improved Scenario over Energy in the Water System in the Baseline Scenario** indicator, which measures the energy that is not necessary to serve as an input on the water system on the improved scenario (in comparison to the baseline scenario) and that is not also necessary to be compensated by external energy sources (both hot and cold utilities and recirculated heat streams).

At the light of the presented verifications, it is possible to affirm that the performance of the optimal point of stream recirculation achieved for the conceptualized systems (which minimizes operational costs the most possible by respecting all the operational constraints) effectively makes possible the reduction of waste streams and the promotion of the recirculation of water and energy to the maximum possible. In this prospect, it may be affirmed that the same set of practices that have been associated to a potential to promote the eco-efficiency of the production processes (through the balanced reduction of both inputs of resources and outputs of wastes) of the analysed plants do also effectively have a similar potential to promote the circular economy character associated to the whole industrial systems.

6.2. Assessment of Strategic Objectives

The driving motive for the project of Water and Energy Integration Systems has been the specific aims that are enunciated on the main sustainability policies of the world (in the case of this work, the policies of the European Union and in an even particularly the policies of Portugal). The sustainability promotion policy that served as the conceptual origin of the WEIS (the main object of study of this work) is the EU strategy for Energy System Integration, primarily its first and third pillars (Energy Efficiency & Circular Economy Nexus and Alternative low-carbon fuels). As this strategy applied the previous principles included in the European Green Deal and the 2050 long-term strategy, the achievement of the aims of the Energy System Integration strategy by the project of WEIS also serves for the same purpose in relation to those policies. Nonetheless, this set of policies have only been framed in a conceptual basis up until this point (in the context of this work). In this prospect, it is necessary to frame the specific numerical results obtained by this work in terms of sustainability promotion-related benefits to the specific aims of the existing policies, so to effectively establish a verification of the potential of the developed concept and derivative case-study results within the objectives to be achieved for the European Union and Portugal.

The aforementioned assessment procedure is interpreted as a manner to achieve the contextualization of the results of this work within the social dimension of the concept of sustainability, as up until this point the focus have been the economic and environmental aspects. In a further perspective, and in a sense the finalize the assessment procedure, a framework of the results within the most recent social issues related to energy and water, namely the ongoing energy crisis and water scarcity (that was particularly aggravated in the summer times of the most recent years of 2022) and 2023, is set to be performed.

6.2.1. Framework of Sustainability Policies Aims

At the light of the requirements for to conjointly promote low-carbon and circular economies and the improvement of water efficiency, the Roadmap for Carbon Neutrality 2050 (RNC2050) [76] and the *Programa Nacional para o Uso Eficiente da Água* (PNUEA) [77] have been proposed as guiding instruments in Portugal. These two strategies are based on the delineation of specific objectives for all the end-use sectors, with RNC2050 containing specific guides for a set of subsectors of the whole industrial sector. The obtained results for the approached case-studies shall reflect those specific aims so to allow one to consider that the elaborated project is capable to achieve the strategic objectives delineated within the policies of the country in which the industrial sites are based.

In respect to the energy use and the promotion of low-carbon energy systems, the RNC2050 has proposed a detailed trajectorial strategy for the industrial sector, in which specific aims for the energy intensity within this end-use sector are proposed for future reference years. These energy intensity levels may be compared to ones determined for the baseline and improved scenarios of the plants. For the side of water efficiency, the PNUEA has proposed a specific efficiency aim to be achieved for the industrial sector for the reference year of 2020, as an improvement of a previous attained objective referent to the year of 2009. The variation between these two levels may be thus compared with the variation obtained for freshwater consumption in the approached water systems. In Table 6-7, the energy intensity levels for the plant and the ones proposed in RNC2050 are presented. In Table 6-8, the water consumption and efficiency levels for the plant and the ones proposed in PNUEA are presented.

Table 6-7. Energy intensity levels for the Plants and relative to RNC2050 specific objectives

Energy Intensity Levels for the Case-study 1 Plant (MJ/€)		
Baseline Scenario	**Improved Scenario**	**Relative Reduction**
14.15	12.15	14.12%
Energy Intensity Levels for the Case-study 2 Plant (MJ/€)		
Baseline Scenario	**Improved Scenario**	**Relative Reduction**
14.15	12.56	11.20%
Energy Intensity Levels within RNC2050 (MJ/€)		
2020 Reference Year	**2030 Reference Year**	**Relative Reduction**
96.27	75.47 | 65.78	21.60% | 31.67%

Table 6-8. Water consumption levels for the water system within the Plants and relative to RNC2050 specific objectives

Water consumption Levels for the Water System within the Case-study 1 Plant (dam^3/year)		
Baseline Scenario	**Improved Scenario**	**Relative Variation**
10.78	8.22	23.71%
Water consumption Levels for the Water System within the Case-study 2 Plant (dam^3/year)		
Baseline Scenario	**Improved Scenario**	**Relative Variation**
6.73	4.14	38.57%
Water efficiency target levels for the Industrial sector (PNUEA)		
2009 Reference Year	**2020 Reference Year**	**Relative Variation (Water Input Levels)**
77.5%	85.0%	8.82%

As may be verified in Table 6-7, the energy intensity levels in respect to the baseline scenario for the plants are significantly inferior to the ones corresponding to the 2020 reference year. Such may be attributed to the relativity low representativity in terms of energy consumption of the ceramic industry in Portugal in relation to the other sectors (as has been delineated in section 2.7). Nonetheless, such comparison is relevant to evaluate the pairing of the objectives of the industrial stakeholders with the aims proposed in a country and sectorial level. As may be observed in Table 6-7, the reduction of energy intensity at plant-level is considerably inferior to the reduction obtained by comparing the levels for the reference years of 2020 and 2030. Such prospect reinforces once more the need for the implementation of complementary energy efficiency improvement measures within the approached plants.

In respect to the levels of freshwater consumption in the approached plants, the benchmark comparison has been performed through the comparison of the freshwater input in each one of the water systems and the water efficiency target levels for the reference years of 2009 and 2020 mentioned in PNUEA (namely the ones pointed out for industry in general). In this case, such comparison is performed by comparing the relative water use reductions obtained for case-studies 1 and 2 and the variation between the corresponding water input levels to the water efficiency levels of 77.5% and 85.0% respectively (similar to the relation between useful energy and supplied energy, it is assumed that the useful quantity of water does not variates and that the total input of water is varied). As may be verified by the analysis of the values present in Table 6-8, the relative water reduction levels obtained for each case-study are significantly higher than the corresponding value determined from the reference values present in PNUEA. Such high difference may be attributed to the superior capacity of the WEIS related to stream recirculation, and thus the water and energy use-related benefits promoted by the implementation of these systems. In this case, such may be attributed to a significantly higher level of water recirculation within the conceptualized water system in comparison to other projected and existing systems. Such recirculation of water streams not only allows the minimal input of hot and cold utilities in the system but also the total freshwater input to be decreased.

6.2.2. Framework of Energy Crisis and Water Scarcity

The development of the present work emerged in a period of history marked by the verification of severe social issues related to the decrease of the availability of determinate natural resources and economic crisis provoked by the COVID19 pandemic and the Russia-Ukraine War [37]. In the context of the areas of actuation inherent to this work, namely on the ones related to energy and water management, it is relevant the analysis of the impact of the ongoing global energy crisis and water scarcity on the actual obtained results.

The present energy crisis asserts essentially on the pillar of the gradually rising energy prices (particularly severe on the case of natural gas), which is directly related to the existing cuts of energy source supply provoked by the War and the economic rebound phenomenon emerged in the follow-up of the pandemic. These gradually rising energy prices have been provoking significant inflation rises, which in its turn have been provoking an augment of economic discomfort by society in general [396]. Simultaneously to this event, several regions of the world have been facing the depletion of water resources availability, an issue that has been particularly strong in Europe in the years of 2022 and 2023 [397]. While for the former issue the promotion of energy efficiency improvement measures allied to renewable energy and alternative fuel integration has been regarded as keys for the solving of it, for the latter the promotion of improved water management techniques in end-use sectors has been similarly pointed as a solving method. The concept of Water and Energy Integration Systems introduced in this work primarily approaches the reduction of both energy and water, thus by hypothesis approaching the development of methods for the solving of the two aforementioned issues.

With the aim to establish a connection between the ongoing societal phenomena with the reality of the case-studies approached in this work, it is necessary to perform a comparison of the determinate indicators calculated from the obtained results considering the implications of the aforementioned issues. For the impact of the ongoing energy crisis, it was selected an analysis method in which the total cost levels associated to natural gas and electricity for both the baseline and improved scenarios and considering the prices for the reference years of 2021 and 2022 are compared. For the assessment of the impact of water scarcity, it was selected a method based on the determination of the water stress, which is calculated by the ratio between freshwater consumption and water availability (this last is determined through an estimation based on the actual water availability in the region in which the case-studies plants are installed) [398]. The described analyses are respectively presented in the sequence of Tables 6-9 and 6-10.

Table 6-9. Determination of Energy prices for the reference years of 2021 and 2022 and for the baseline and improved scenarios

Year	Baseline Scenario (BS)	Improved Scenario (IS)	Relative Savings	Relative difference between BS's	Relative difference between 2022 BS and 2021 IS
Case-study 1 Plant					
Natural Gas-associated costs					
2021	2.55	2.32	8.80%	64.62%	67.74%
2022	7.19	6.56			
Electricity-associated costs					
2021	2.42	2.23	8.01%	11.31%	18.42%
2022	2.73	2.51			
Case-study 2 Plant					
Natural Gas-associated costs					
2021	2.55	2.34	7.92%	64.62%	67.42%
2022	7.19	6.63			
Electricity-associated costs					
2021	2.42	2.36	2.83%	11.31%	13.82%
2022	2.73	2.66			

Table 6-10. Determination and comparison of water stress levels for the case-study plants

Baseline Scenario		**Improved Scenario**	
Water stress in relation to the Water System within the Case-study 1 Plant			
91.57%		69.86%	
Water stress in relation to the Water System within the Case-study 2 Plant			
57.19%		35.13%	
Benchmark Water Stress Levels [398]			
Low scarcity	**Moderate scarcity**	**Significant scarcity**	**Severe scarcity**
Less than 10%	10 – 20%	20 – 40%	More than 40%

As may be observed by the analysis of the results presented in Table 6-9, the total energy-related costs obtained for the two reference years presented considerable deviations, which are much more significant in the case of natural gas, whose corresponding unitary price rise from 2021 to 2022 was about 183% for the case of Portuguese industry. In Table 6-9, the obtained relative savings are presented to be compared with the relative difference between 2021 and 2022 baseline scenario and between 2022 baseline scenario and 2021 improved scenario. At the light of the obtained relative savings, it is possible to verify that for natural gas the obtained savings are highly lower than the values obtained for the two mentioned relative differences, with this being verified for both case-studies. For the case of electricity, such disparity is not so high, although it is still considerable in case-study 2. Taking into account the verified disparities, it may be affirmed that although the implemented energy efficiency improvement measures have been proved to be effective in the context of overall promotion of eco-efficiency and the circular economy character associated to the production processes with the analysed plants, the obtained energy use reduction levels do not produce sufficient reduction at the level of operational costs to fully compensate for the rising energy prices. At the light of such affirmation, it may be once more brought the requirement to further propose and implement complementary improvement measures at the level of energy use, with the aim to approximate the present energy-related costs to the ones that are estimated in the corresponding hypothetical 2021 scenarios. While for electricity it passes by the implementation of additional measures related to the use of electricity (such as the ones related to the improvement of the operation of electric motors and involved systems), for natural gas such approximation passes by more extensive and complex energy management projects, namely the ones which involve the refurbishment of the plant operation to include alternative and potentially more economically viable fuels.

In respect to the assessment of the implications inherent to the water scarcity phenomenon, it is possible to verify by the analysis of the results presented in Table 6-10 that freshwater consumption within the water system of the plants is significantly high in comparison to the estimated levels of average water availability for both case-studies. In this prospect, it may be affirmed that the analysed water systems are operating in a level that significantly surpass the limit from which these generate local water stress, which may potentially be a cause of further unavailability of freshwater on local communities. Taking into account that the analysed water systems do not encompass all the water-using units within the analysed plants, the implications of such observations are aggravated (particularly for case-study 1, in which the baseline scenario corresponds to a 91.57% water stress). For case-study 1, the improved water management achieved in the improved scenario is not even sufficiently to alter the operation point from water stress level, being maintained in the severe scarcity level. For case-study 2, it is possible however to generate an alteration from severe scarcity to significant scarcity. At the light of these observations, it is possible to affirm that further water management techniques are required to be implemented for furtherly diminish the risk of water stress levels of the analysed systems. Such techniques may pass by the diversification of feed water sources. Furthermore, and at the light of the existing benchmark resource use levels (in which the ceramic industry is inserted in the sectors of modest water use in comparison to others) it is possible to affirm that, although the analysed plant may be associated to relatively low water consumption in comparison to other sector plants, in the context of the geographical region in which the plants are installed the overall use of water as a resource is much more representative.

Final Considerations

As the economic and environmental viability of the conceptualized Water and Energy Integration Systems (WEIS) installations have been reinforced by the verification of the eco-efficiency and circular economy character of these installations and the approximation of the case-studies proper results to strategic aims have been proved, it is proved the existence of necessary conditions for the consideration of the conceptualized projects as being sustainable. In relation to the approximation to strategic aims, it may be assumed that the compliance of the case-studies' results with the analysed indicators also leads to the insurance that social-related benefits are also achieved although not being directly calculated, as assumed afore. The social-related benefits that are assumed to be promoted are based on the following aspects (which are prominently delineated in RNC2050 [76]):

- **Promotion of a socially fair and efficient energy transition**: the conceptualized WEIS installations do not require additional investment on land except the one that is already used for plants to be installed and it requires investment costs that are assumed to be allocated from the industrial stakeholders, with the existence of government incentives;
- **Reinforcement of the competitiveness of the regional and industrial economies**: for both case-studies, payback periods of less than the most favourable and acceptable limit of 3 years and maximum acceptable limit of 5 years are obtained, which is significant that a considerable margin of total savings is possible to be allocated to the promotion of other benefits and the limits to which the commissioned installations are considered to be economic viable are nevertheless not surpassed;
- **Promotion of the creation of work positions**: this may be regarded as one of the aforementioned benefits;
- **Improvement of air quality and overall human health**: while the improvement of air quality is secured by the reduction of waste gas emissions (as evidenced by the final simulation results obtained for the case-studies), the improvement of human health may be secured by the combination of this benefit and the improvement of the quality of discharge water (which may be evidenced by the null level of the discharge water obtained for the case-studies), as well as the relative increase of water availability.

The insurance of the existence of these benefits is thus a necessary and sufficient condition to ensure the sustainability promotion character of the conceptualized WEIS installations.

7. Conclusions and Future Work

The present work has been developed with the assumption that the already existing operation of plants within process industries has associated a significant potential of improvement in terms of the use of energy and water. The improvement of these resources use is furtherly assumed to be possible to be performed simultaneously and in a similar manner. It is certain that several types of designations exist in literature to design industrial systems that include several unit operations and the interconnections between these. In general, these systems are conceptualized bearing in mind the reduction of energy and water inputs (different types of systems approaching the improvement of these resources use simultaneously or in separate) and the reduction of the contaminants contained in the streams resulting from energy and water-using processes.

In this work, a new concept designated as Water and Energy Integration Systems (WEIS) has been introduced. This concept primarily integrates the previously introduced concept of water allocation and heat exchanger networks (WAHEN), which are conceptualized according to the Combined Water and Energy Integration (CWEI) method, with the most common practices of waste heat recovery from the streams at the outlet of combustion-based processes. The conceptualization of WEIS has been the central objective of this work in terms of Engineering project development. The arrival point for this work has been having these systems conceptualized in a phase of design, in which the real data from combustion-based processes and water-using units from selected plants is gathered and use to estimate benefits that potentially result from the implementation of these systems. Two case-studies have been selected the proposed objective achievement both inserted in the framework of the Portuguese ceramic industry, which in this case has been selected owing to a convenience of a simultaneous availability of data and the placement of this sector within process industries with a considerable quantity of streams to be valorised and sufficiently robust energy and water consumptions to be potentially reduced. Since these are types of systems that may be implemented for all the sectors of process industry in general as long as combustion-based processes and water-using units producing wastewater streams exist in the plants of these sectors, the results obtained for indicators translating the achievement of the aforementioned benefits may serve as a benchmark for the analysis of similar systems in other plants.

The methodology used in this work to study the implementation of the new conceptual systems is based on the development and further use of simulation and optimisation models. These models are part of a new customised computational tool designated as ThermWatt. The main simulation modules of ThermWatt have been developed using the Modelica language, while secondary modules related to steady state-based optimisation models have been developed using the Python language.

The concept of Water and Energy Integration Systems (WEIS) and the ThermWatt computational tool are two innovative assets which served as a basis for the development of this work. The WEIS concept has been created subsisting on the existing industrial practices of recycling, reuse and by-pass and a set of technologies that conjointly implemented produce energy and water-related benefits, namely technologies for waste heat recovery, thermal energy storage, heat-driven wastewater treatment and energy recovery from water and wastewater. In the framework of the studied technologies, two different WEIS configurations were conceptualized: the standard (steady-state based) WEIS configuration and the dynamic-based WEIS configuration (which considers the transient mode of operation of the thermal energy storage units). These configurations subsist on the concept of superstructure, being the most general formulations to be adapted for the case-studies' systems with these in its turn being analysed in terms of the most suitable counterpart technologies and the effectiveness of stream recirculation.

The ThermWatt computational tool, in its turn, subsists on new models that use essentially newly developed software code and that adapt existing modelling and optimisation methods. The practical application of the ThermWatt tool (which in this work serve as the tool for the virtual realization of WEIS projects) subsists on the use of equipment models that are assembled in a system-level model which considers all the necessary and planned interconnections between components. In this prospect, a set of component models have been developed to virtually represent the existing plant operations, such as combustion-based processes, water-using processes and improvement technologies. These models have been tested using real plant and literature data in model validation phase. The model validation procedure has been proved successful, in terms of numerical results, with all the sets of variables presenting deviations of less than 5%. Moreover, for variables whose change with time has been set to be analysed (in the perspective of dynamic simulation), the reference and simulated variation profiles of such variables present a reasonable correspondence for all cases.

In the follow-up of the afore detailed model development, a set of simulation models were created for the two proposed case-studies. For each case-study, a set of three system-level models were developed, one for the baseline scenario and two for different improved scenarios, corresponding to two different WEIS scenarios adapting the most general configurations. While for case-study 1 the standard WEIS configuration is adapted, for case-study 2 the dynamic-based one is implemented due to existence of batch units in the plant. For each configuration, two sub-scenarios were furtherly developed: one considering the electricity generation as a source of electric energy savings and another considering the use of it for hydrogen production. The whole sets of scenarios for each case-study have been compared in terms of the total operational costs, in which the summation of the costs associated to natural gas, electricity and freshwater consumption have been considered. From the performance of each scenario analysis, it was proved that the use of produced electricity for electric energy savings was favourable in comparison to its use for hydrogen production, with a total operational costs reduction of about 0.744 and 0.490 million €/year having been obtained for case-studies 1 and 2, respectively.

The conceptualization of WEIS scenarios and corresponding system-level models served as the founding for the development of optimisation models, which serve as counterparts for the previously developed simulation models. Being duplicates of the previous models in terms of physical phenomena modelling, these models had to fulfil the two main objectives of obtaining the optimal points corresponding to the minimized total operational costs for each case and the numerical correspondence between the previously obtained simulation results and newly obtained optimisation results. A complex procedure for the solving of the proposed optimisation problems has been taken for each case-study. While for case-study 1 only one non-linear programming (NLP) model has been developed (using the non-linear programming approach), for case-study 2 two models have been developed, one using the non-linear programming approach and the other using the dynamic programming approach. This procedure was taken to fulfil two different optimisation modelling requirements, since the conceptualized WEIS may be disaggregated for this end in the water system that operates essentially in a steady state perspective and the thermal process system that encompassed the TES unit. This complex procedure converged on the integration of the obtained results on the developed case-studies' simulation model framework, which furtherly allowed the final numerical results to be used for post-processing. This post-processing was based on the performance of the determination of the economic and environmental impact reduction viability associated to the WEIS projects. While the economic viability assessment was performed by estimating the payback period associated to each project, the environmental impact reduction assessment was based on the determination of the absolute equivalent carbon dioxide emissions reduction. For case-study 1, a payback time of about 1 year and 10 months and a 2.42 kton $\mathrm{CO_{2,eq}}$/year reduction were estimated. In its turn, for case-study 2, a payback time of about 2 years and 10 months and a 1.76 kton $\mathrm{CO_{2,eq}}$/year reduction were estimated. In the case of economic viability assessment, the estimated payback times for both case-studies may be considered reasonable, with both being lower than a than 3 years benchmark. The obtained levels of $\mathrm{CO_{2,eq}}$ emission reduction may in its turn are considered significant based on the reference values for similar plants (a maximum of about 0.722 kton $\mathrm{CO_{2,eq}}$/year).

The optimisation modelling framework developed for this work allowed the creation of a basis of model to be used and adapted for further cases, either technologies or sectorial case-studies. This work firstly approached the higher coverage of this type of superstructure optimisation models from its existing form to the application of these for the reality of specific sectorial case-studies (in this case, the ceramic industry). Furtherly, the developed optimisation framework considered the specific requirements associated to the existing industrial processes. On the side of the conceptualization of thermal process system, the optimisation framework considered the different requirements associated to the presence of continuous or batch energy-using units, as it has been verified for case-studies 1 and 2, respectively. On the side of water systems conceptualization, the optimisation framework has been prepared to consider different quality levels of water streams, which in this case is verified by the fact that its application to a single contaminant problem (case-study 1) generates results in an equally effective manner compared to a multi-contaminant problem (case-study 2).

At the point of view of sustainability assessment, the viability in terms of economic and environmental feasibility has been proved through the aforementioned evaluations. Nonetheless, it is to note that two objectives that have been initially proposed in this work and that have been delineated by hypothesis with the concept of WEIS have been the potential to promote the eco-efficiency of the production processes within the analysed plants and the circular economy character of the conceptualized systems. As such, a set of indicators have been calculated for each one of the case-studies and the aforementioned aspects.

The results obtained from the determination of these indicators effectively reinforce the conclusions pointed out in the economic and environmental impact reduction assessment, having been proved the potential of the WEIS projects for both eco-efficiency promotion and the circular economy potential of these. It has been also noted that these two aspects associated to the conceptualized systems may be significant and furtherly promoted through the exploitation of interdependencies between the to-be-valorised heat stream recirculation and water stream recirculation, as part of the water-energy nexus character that has been taken as a starting point for the creation of the WEIS concept. The results for these indicators proved that the conceptualized WEIS projects may be considered generally robust in terms of eco-efficiency, potential for circular economy and potential for achieving strategic objectives, with an improvement of 6.46% and 4.00% for the aggregated eco-efficiency indicator obtained for case-studies 1 and 2, respectively, a zero-water discharge for both case-studies and a level of 8.58% and 6.69% of recycled heat over total energy consumption. Nonetheless, the performed assessment also proved that additional measures, in particular those related to energy efficiency improvement, are necessary to be possible to determinate indicators, such as specific energy consumption levels and GHG emission intensities, to be comparable with benchmark values for the approached sector of the ceramic industry.

Furtherly, an assessment subsisting on the comparison of similar indicators to those determined in the most recent sustainability policies has been performed with the aim to assess the actual positioning of the projected improved scenarios in terms of benchmark values mentioned to be possible to be achieved through the adequate implementation of those policies. Throughout the comparison of the energy intensity levels for the industrial sector mentioned in the Portugal Roadmap for Carbon Neutrality 2050 (RNC2050) and the water consumption levels referred in the *Programa Nacional para o Uso Eficiente da Água* (PNUEA) with the corresponding ones from both case-studies, it has been proved the achieved benefits are in line with those mentioned in the existing sustainability policies in terms of order of magnitude of the obtained values of the two analysed indicators. Moreover, an assessment based on the study of the impact of the most recent social phenomena of the energy crisis and water scarcity occurring in several countries of the European Union was performed. For the case of the study of the energy crisis-related implications, it was verified that the proposed energy efficiency improvement measures are unable to make possible for the energy-related operational costs determined for the reference year of 2022 to be compatible with the ones hypothetically obtained using 2021 unitary energy prices (a situation that is particularly sever for the case of natural gas). For the case of the study of the water scarcity implications, it has been proved that the proposed water management configuration is generally not sufficient to solve issues related to water stress assuming an average level of water availability for the region in which the plants are installed. This last verification is in opposition of starting point assumptions taken for the approached sector, which is associated to modest water consumption levels in comparison to other process industry sectors. This denotates that relative water scarcity is more effective to be analysed as a local problem rather than most generally a water supply system such as it occurs for energy supply (owing to the fact that the supply of energy resources subsists on standardized control and monitoring automatically performed for an interconnected nation-wide energy system, while for water it depends the availability of this resource for the region, as a similar system to one of energy still does not exist).

The whole modelling and post-processing assessment led to the creation of a new manner of developing Engineering projects for the plants of process industries, namely in respect to the integration of several types of technologies with the ultimate aim to achieve a balanced reduction of the economic and environmental burdens associated to water and energy use. The most recently commonly implemented concepts of eco-efficiency and circular economy have been used in conceptualization phases and its effective verification has been proved in the context of industrial case-studies. As such, the present work had contributed on a new perspective on the exploitation of the interdependencies between energy and water resources as encompassed by the concept of water-energy nexus, throughout the consideration of to-be-valorised energy and water streams as having similar properties in terms of recirculation and the projected implementation of all potential technologies for a same industrial case.

Future Work

The development of the future work inherent to the own development aspects of the present thesis focus on the two innovative assets that serve as the thematic structure of the work: the Water and Energy Integration Systems (WEIS) concept and the ThermWatt computational tool.

In respect to the Water and Energy Integration Systems (WEIS) concept and related analysis, the following aspects may be attended to:

- The integration of post-combustion carbon capture technologies in further WEIS configurations;
- The assessment of environmental burden reduction-related benefits at the level of specific water contaminant reduction;
- In relation to desalination as wastewater treatment technologies, the proposal of technologies for the valorisation of concentrate streams (energy and salt recovery-related benefits).

In respect to the ThermWatt computational tool, the following aspects may be attended to:

- The further development of combustion-based processes simulation models (namely considering a highest level of the modelling of the heat transfer and reaction-based phenomena within these processes);
- The further development of thermal energy storage technologies simulation models (in particular thermochemical energy storage units);
- The further development of wastewater treatment technologies simulation models (in particular the more conventional technologies based on biological treatment and membranes);
- The further development of simulation models for energy recovery from water/ wastewater technologies (namely the most traditional technologies and thermochemical water splitting as an alternative to Electrolysis);
- The analysis of the implementation of multi-objective programming (MOP) models as an alternative to the developed non-linear programming (NLP) models for the purpose of the solving of the presented optimisation problems (and similar ones for different case-studies WEIS);
    - These MOP models may subsist bi-objective (or more-than-two) optimisation, in which the parcels of the total operation cost functions (as enunciated in this work) are separated (for instant, for the parcels related to natural gas, generated electricity and water).

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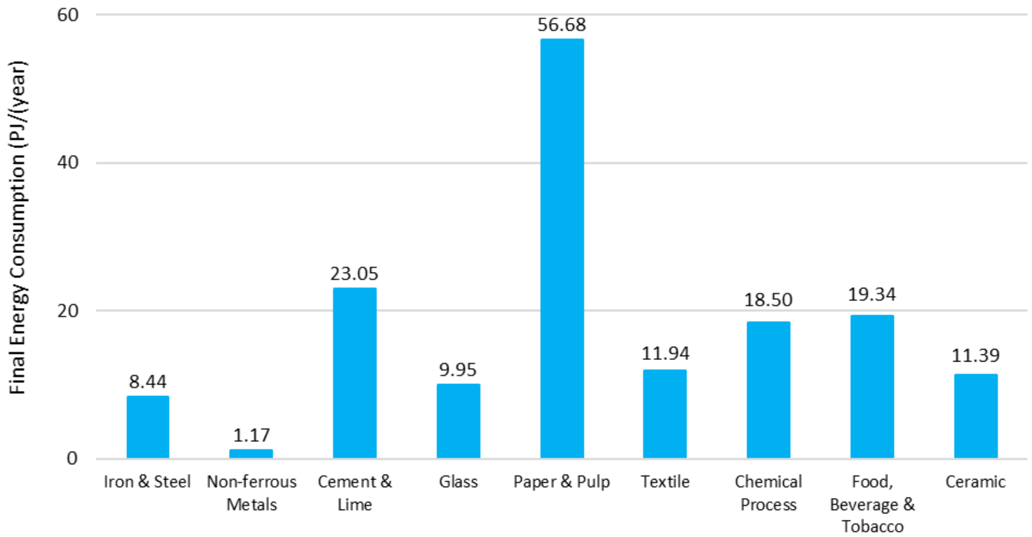
Appendices

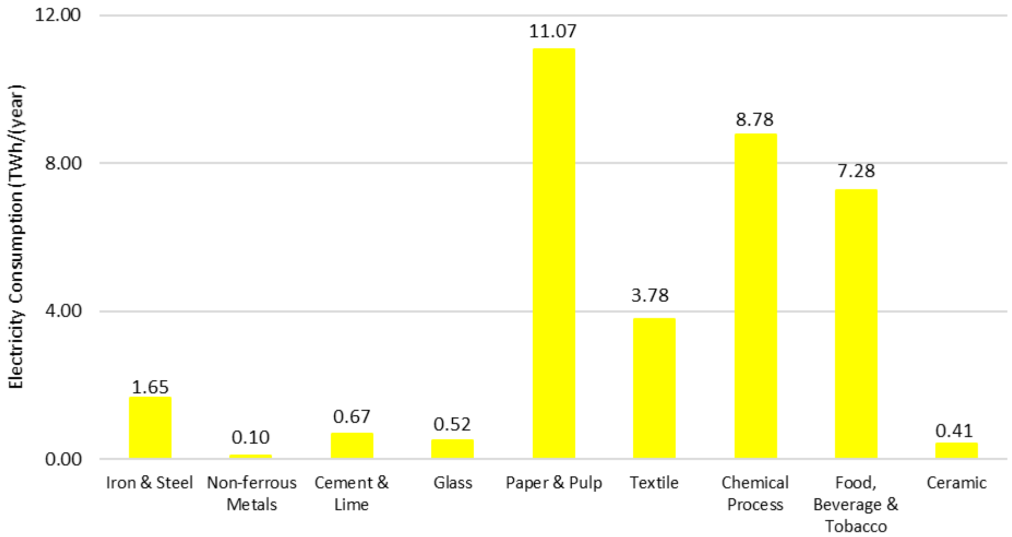
In this section, appendices for this thesis are presented. The sequence of these appendices present information from which the main contents afore presented subsist on. These either give a theoretical or a practical basis or miscellaneous topics associated to the whole modelling and post-processing work performed for this thesis.

A1. Absolute Water and Energy Consumptions

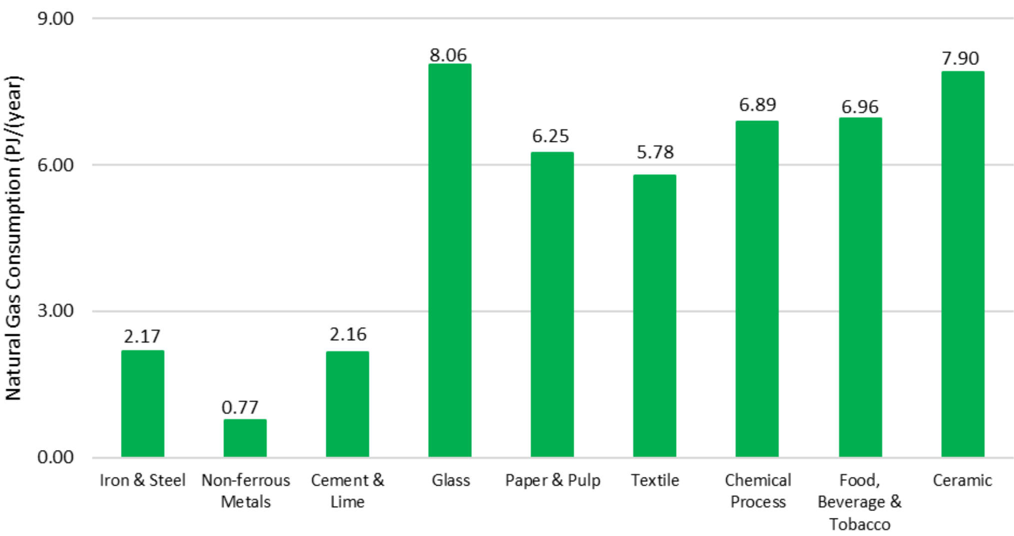
The absolute water and energy consumption for the industrial sectors selected to be analysed on a statistical basis are graphically presented in the sequence of Figure A1 – A3.



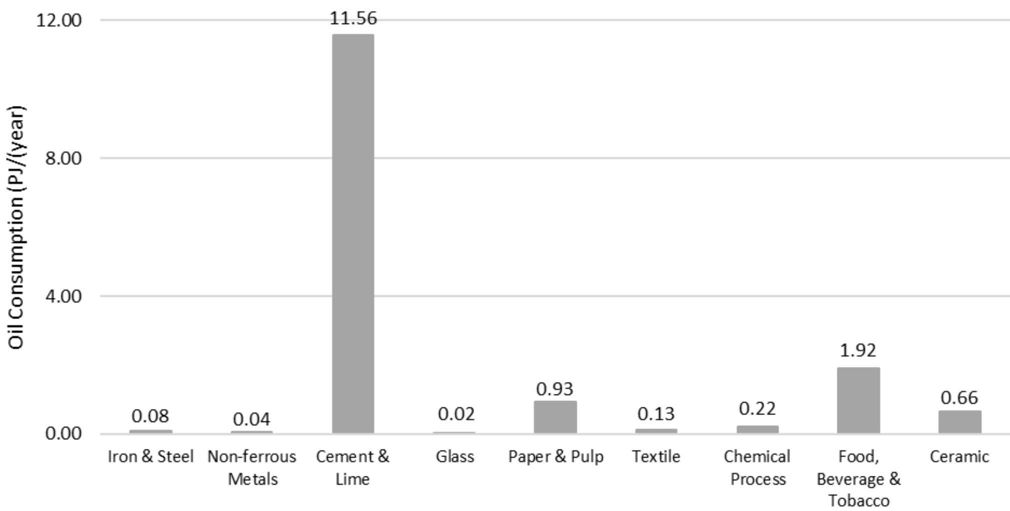
a)



b)



c)



d)

Figure A1. Final energy consumption levels for nine process industry sectors in Portugal: a) Final Energy Consumption, b) Electricity Consumption, c) Natural Gas Consumption, d) Oil Consumption

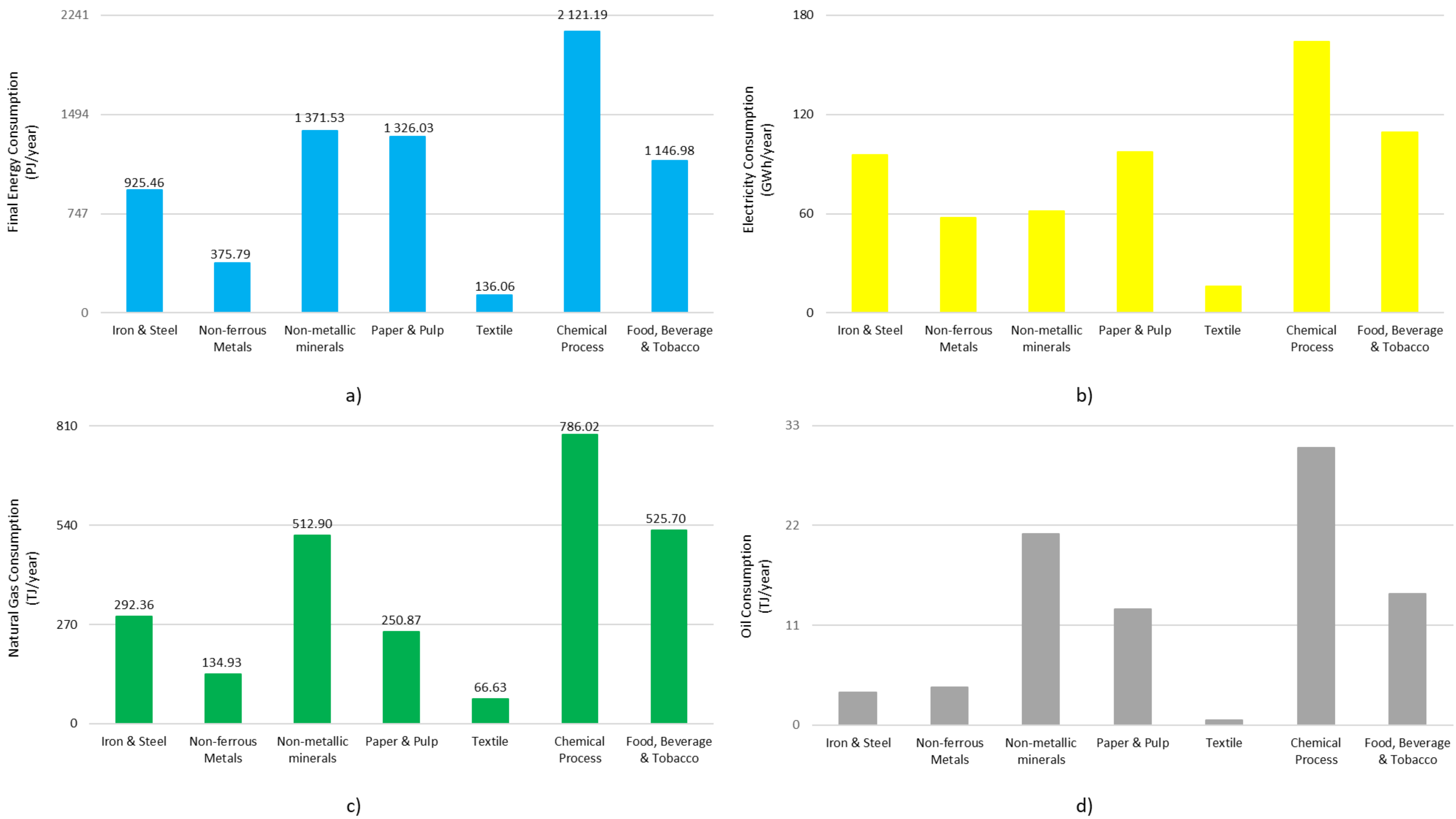


Figure A2. Final energy consumption levels for seven process industry sectors in the European Union: a) Final Energy Consumption, b) Electricity Consumption, c) Natural Gas Consumption, d) Oil Consumption

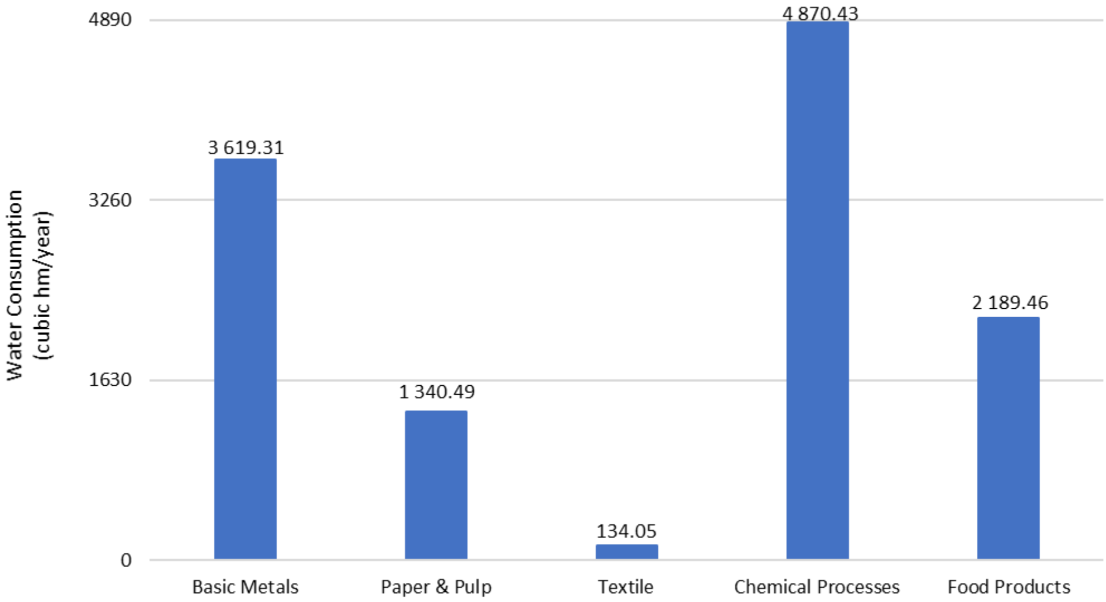


Figure A3. Water consumption for five sectors of the process industry in the European Union

A2. Derivation of Thermal Energy Storage equations for cylindrical-type geometries

For the case of a cylinder shape, and in the case of the inexistence of heat generation, the equation for conductive heat transfer in the transient state may be resumed to equation (A1).

$$\frac{1}{r} \cdot \frac{d}{dr}\left(r \cdot k \cdot \frac{dT}{dr}\right) = \rho \cdot C_P \cdot \frac{dT}{dt} \tag{A1}$$

The consideration of equation (A1) in a simulation model (such as the ones to be developed with the Modelica language) requires further adaptation. Such procedure is necessary to allow the application of discretization methods, such as the finite difference method (FDM). In this case, the use of discretization methods is necessary for the determination of spatial-related quantities of heat conduction variables. In the case of the use of the Modelica language, for time-related quantities, such procedure is not necessary, as Modelica-based environments are set to automatically calculate time-dependent derivatives. The further development of equation (A1), attending to the application of the derivative product rule, results in equations (A2).

$$k \cdot \frac{1}{r} \cdot \left(\frac{d}{dr}(r) \cdot \frac{dT}{dr} + r \cdot \frac{d^2T}{dr^2}\right) = \rho \cdot C_P \cdot \frac{dT}{dt} \tag{A2}$$

The further development of equation (A2) (considering the solving of the derivative parcels) results in equation (A3), respectively.

$$k \cdot \left(\frac{1}{r} \cdot \frac{dT}{dr} + \frac{d^2T}{dr^2}\right) = \rho \cdot C_P \cdot \frac{dT}{dt} \tag{A3}$$

Considering the assumption of constant thermal diffusivity for the PCM phase, equation (A3) may be reformulated to equation (A4).

$$\alpha \cdot \left(\frac{1}{r} \cdot \frac{dT}{dr} + \frac{d^2T}{dr^2}\right) = \frac{dT}{dt} \tag{A4}$$

A3. Derivation of the Equations for the Determination of PCM Properties (Melting Phase)

The melting phase of phase change materials (PCM) is associated to a considerable complexity in terms of the determination of the properties associated to the material. While in the solid and liquid phases, the properties that characterize the PCM, namely the specific heat capacity, the thermal conductivity and density, in the melting phase these properties highly vary according to the range of temperatures of the melting phase. The application of the apparent specific heat capacity method for the determination of these properties during the melting subsists on the application of models for the variation of the specific heat capacity and the other properties with temperature. In Figure A4, the variation of the apparent specific heat capacity with the PCM temperature is graphically presented.

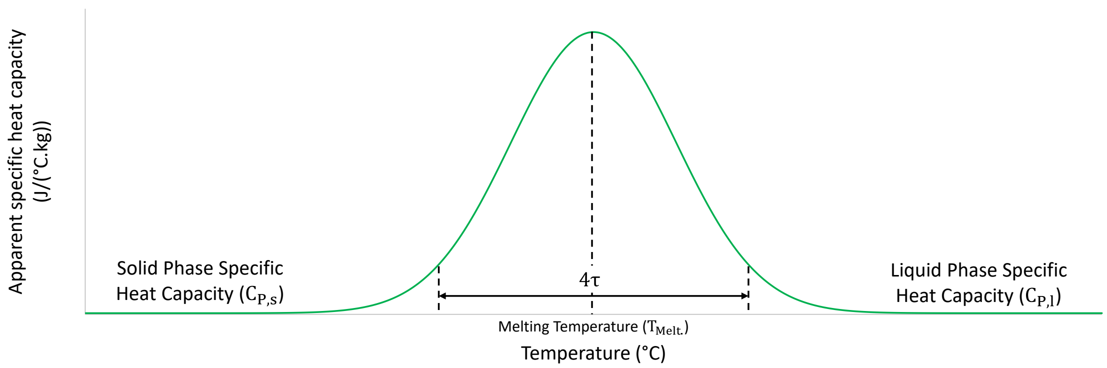


Figure A4. Variation of apparent specific heat capacity with temperature for a generic PCM (Temperature melting range)

The computation of the value specific heat capacity and the other properties for a given value of PCM temperature is based on the application of analytical equations, as presented in the sequence of equations (A5) – (A7).

$$C_{P,app.} = \frac{\Delta h_{Cond.}}{(2 \cdot \pi)^{0.5} \cdot \tau} \cdot \exp\left(\frac{-(T - T_S)^2}{2 \cdot \tau^2}\right) + C_{P,S} + \left(C_{P,L} - C_{P,S}\right) \cdot 0.5 \cdot \mathrm{erf}\left(\frac{(T - T_S)}{\sqrt{2} \cdot \tau}\right) \quad \text{(A5)}$$

$$k = k_s + (k_l - k_s) \cdot 0.5 \cdot \mathrm{erf}\left(\frac{(T - T_S)}{\sqrt{2} \cdot \tau}\right) \quad \text{(A6)}$$

$$\rho = \rho_s + (\rho_l - \rho_s) \cdot 0.5 \cdot \mathrm{erf}\left(\frac{(T - T_S)}{\sqrt{2} \cdot \tau}\right) \quad \text{(A7)}$$

In the context of the development of computational models, such as the developed with the Modelica language in this work, the error function (erf) may be conveniently computed through the use of approximations, such as the ones presented in equation (A8).

$$\operatorname{erf}\left(\frac{(t - \mathrm{T_S})}{\sqrt{2} \cdot \tau}\right) = \left(1 + \left(-1 + \frac{2}{1 + \exp\left(-2.5 \cdot \left(\frac{(\mathrm{T} - \mathrm{T_S})}{\sqrt{2} \cdot \tau}\right)\right)}\right)\right) \tag{A8}$$

A4. Characterization of the Properties of Working Fluids and Heat Storage Materials

The modelling of fluids and heat storage materials considered in this work subsist on the determination of physical properties. While the ThermWatt Modelica library contains packages for fluids such as the ones mentioned in chapter 3 (as adaptations of the packages present in the ThermoPower library), several packages for the computation of material properties had to be newly developed. These are, for instance, the package for the organic working fluid considered for the Organic Rankine Cycle (ORC) systems and the considered PCM material for case-study 2. For the most fundamental considered fluids (natural gas, hydrogen, air/ exhaust gas and water), a set of assumptions have been performed for the determination of properties in which the main package (such as IF97 for water) is inaccessible owing to technical limitations associated to model development. Due to a reason of convenience of model development, the determination of a set of properties have been simplified (for instance the relation between temperature and specific enthalpy for water and air/ exhaust for the optimisation models). These properties and determination methods are presented in the sequence of Table A1 – A3.

Table A1. Characterization of the considered organic working fluid (NOVEC649)

Property	Value
Melting Temperature (ºC)	52
Density (kg/m^3)	1610
Saturated liquid specific enthalpy (J/kg)	21000
Saturated vapour specific enthalpy (J/kg)	109000
Specific heat capacity (J/(ºC.kg))	1103
Molar mass (kg/mol)	0.31604
Critical Temperature (ºC)	168.66
Critical Pressure (Pa)	1869026.5831
Critical Molar Volume (m^3/kmol)	0.5208

Table A2. Characterization of the considered phase change material (PlusICE Organic Range A73)

Property	Value
Melting Temperature (ºC)	73
Density (kg/m^3)	890
Latent enthalpy (J/kg)	225000
Specific heat capacity (J/(ºC.kg))	2200
Thermal conductivity (W/(m.ºC))	0.23
Maximum operational temperature (ºC)	250

Table A3. Characterization of the primarily considered fluids

Fluid	Property	Value/ Formula
Natural Gas	Lower heating value (GJ/kg)	0.0451
Hydrogen	Lower heating value (GJ/kg)	0.12021
	Molar mass (kg/mol)	0.002016
Air/ Exhaust gas	Temperature – Specific	$\mathrm{h(kJ/kg)} = 1.0700 \cdot \mathrm{T(°C)} + 265.1454$ (A9)

	Enthalpy relation		
Water	Density (kg/m^3)	999	
	Molar mass (kg/mol)	0.0180152	
	Temperature – Specific Enthalpy relation	$\mathrm{h(kJ/kg)} = 4.1887 \cdot \mathrm{T(°C)} + 0.0259$	(A10)

A5. Case-study 1 Optimisation Model (Python Code)

The NLP model developed for case-study 1 is presented in Code Listing A1. The association of the defined variables to each stream and WEIS component for case-study 1 is presented in Figure A5 (in which each stream/ component within the WEIS flow sheet is characterized according to its definition in the developed code).

Code Listing A1. Optimisation model for Case-study 1 (Python code)

```
from gekko import GEKKO



# CS1 Model Setup

m = GEKKO() # Initialization
m.options.SOLVER=3 # Definition of IPOPT solver



# Setup of APOPT Solver
m.solver_options = ['max_iter 5000000',
                    'linear_solver mumps',\
                    'mu_strategy adaptive']



# Decision Variables



## Thermal Process System

M1Z = m.Var(lb=0.00,ub=196.50)
M2Z = m.Var(lb=0.00,ub=103.50)

M1 = m.Var(lb=0.00,ub=196.50)
M2 = m.Var(lb=0.00,ub=16284.00)
MA2 = m.Var(lb=0.00,ub=16284.00)
M3 = 20711.70
M4 = m.Var(lb=0.00,ub=20711.70)
M5 = m.Var(lb=0.0,ub=20711.70)
M6 = m.Var(lb=0.00,ub=20711.70)
M7 = m.Var(lb=0.00,ub=16480.50)
M8 = m.Var(lb=0.00,ub=103.50)
MA9 = m.Var(lb=0.00,ub=14351.00)
M9 = m.Var(lb=0.00,ub=14351.00)
M10 = 23583.10
M11 = m.Var(lb=0.00,ub=23583.10)
M12 = m.Var(lb=0.00,ub=23583.10)
M13 = m.Var(lb=0.00,ub=23583.10)
M14 = m.Var(lb=0.00,ub=14454.50)
M15 = m.Var(lb=0.00,ub=44294.80)
M16 = m.Var(lb=0.00,ub=30935.00)




M15A1 = m.Var(lb=0.00,ub=44294.80)
M15A2 = m.Var(lb=0.00,ub=44294.80)
M15A3 = m.Var(lb=0.00,ub=44294.80)
M15A4 = m.Var(lb=0.00,ub=44294.80)

M15MED = m.Var(lb=0.00,ub=44294.80)




MORC = m.Var(lb=0.00,ub=75229.80)
```

```
T1 = 37.00
T2 = 35.00
TA2 = m.Var(lb=35.00)
T3 = 193.18
T4 = 193.18
T5 = 193.18
T6 = 193.18
T7 = m.Var(lb=230.00)
T8 = 37.00
T9 = 41.50
TA9 = m.Var(lb=41.50)
T10 = 93.52
T11 = 93.52
T12 = 93.52
T13 = 93.52
T14 = m.Var(lb=159.30)
T15 = m.Var(lb=93.52,ub=193.18)
T16 = m.Var(lb=159.30)


T15A1 = m.Var(lb=35.00,ub=193.18)
T15A2 = m.Var(lb=35.00,ub=193.18)
T15A3 = m.Var(lb=35.00,ub=193.18)
T15A4 = m.Var(lb=35.00,ub=193.18)

T15MED = m.Var(lb=35.00,ub=193.18)
T15MEDInt = m.Var(lb=35.00,ub=193.18)


TORC = m.Var(lb=35.00)

TORCOut = m.Var(lb=75.00)




h1 = 0.000
h2 = 302.595
hA2 = m.Var(lb=302.595)
h3 = 471.846
h4 = 471.846
h5 = 471.846
h6 = 471.846
h7 = m.Var(lb=511.245)
h8 = 0.000
h9 = 309.550
hA9 = m.Var(lb=309.550)
h10 = 365.213
h11 = 365.213
h12 = 365.213
h13 = 365.213
h14 = m.Var(lb=435.596)
h15 = m.Var(lb=365.212,ub=471.848)
h16 = m.Var(lb=435.596)






h15A1 = m.Var(lb=302.595,ub=471.848)
h15A2 = m.Var(lb=302.595,ub=471.848)
h15A3 = m.Var(lb=302.595,ub=471.848)
h15A4 = m.Var(lb=302.595,ub=471.848)



h15MED = m.Var(lb=302.595,ub=471.848)
h15MEDInt = m.Var(lb=302.595,ub=471.848)


hORC = m.Var(lb=302.595)


hORCOut = m.Var(lb=345.395)
```

```
E = m.Var(lb=0)
E1 = m.Var(lb=0)
E2 = m.Var(lb=0)

EMED = m.Var(lb=0)



qH1 = m.Var(lb=0.00)
qH2 = m.Var(lb=0.00)
qH3 = m.Var(lb=0.00)
qH4 = m.Var(lb=0.00)


qMED = m.Var(lb=0.00)

qMEDLoss = m.Var(lb=0.00)



AH1 = m.Var(lb=0.00)
AH2 = m.Var(lb=0.00)
AH3 = m.Var(lb=0.00)
AH4 = m.Var(lb=0.00)


AHMED = m.Var(lb=0.00)




## Water System



MW1 = m.Var(lb=0.00,ub=1719.73)

MW2 = m.Var(lb=0.00,ub=593.54)
MW3 = m.Var(lb=0.00,ub=596.40)
MW4 = m.Var(lb=0.00,ub=456.79)
MW5 = m.Var(lb=0.00,ub=73.41)

MW6 = m.Var(lb=0.00,ub=593.54)
MW7 = m.Var(lb=0.00,ub=593.54)
MW8 = m.Var(lb=0.00,ub=593.54)
MW9 = m.Var(lb=0.00,ub=593.54)
MW10 = m.Var(lb=0.00,ub=593.54)

MW11 = m.Var(lb=0.00,ub=596.40)
MW12 = m.Var(lb=0.00,ub=596.40)
MW13 = m.Var(lb=0.00,ub=596.40)
MW14 = m.Var(lb=0.00,ub=596.40)
MW15 = m.Var(lb=0.00,ub=596.40)

MW16 = m.Var(lb=0.00,ub=456.79)
MW17 = m.Var(lb=0.00,ub=456.79)
MW18 = m.Var(lb=0.00,ub=456.79)
MW19 = m.Var(lb=0.00,ub=456.79)
MW20 = m.Var(lb=0.00,ub=456.79)

MW21 = m.Var(lb=0.00,ub=73.41)
MW22 = m.Var(lb=0.00,ub=73.41)
MW23 = m.Var(lb=0.00,ub=73.41)
MW24 = m.Var(lb=0.00,ub=73.41)
MW25 = m.Var(lb=0.00,ub=73.41)

MW26 = m.Var(lb=0.00,ub=593.54)
MW27 = m.Var(lb=0.00,ub=596.40)
MW28 = m.Var(lb=0.00,ub=456.79)
MW29 = m.Var(lb=0.00,ub=73.41)

MW26A = m.Var(lb=0.00,ub=593.54)
MW27A = m.Var(lb=0.00,ub=596.40)
MW28A = m.Var(lb=0.00,ub=456.79)
```

```
MW29A = m.Var(lb=0.00,ub=593.54)

MW30 = m.Var(lb=0.00,ub=593.54)
MW31 = m.Var(lb=0.00,ub=596.40)
MW32 = m.Var(lb=0.00,ub=456.79)
MW33 = m.Var(lb=0.00,ub=73.41)

MW34 = m.Var(lb=0.00,ub=593.54)
MW35 = m.Var(lb=0.00,ub=593.54)
MW36 = m.Var(lb=0.00,ub=593.54)

MW37 = m.Var(lb=0.00,ub=596.40)
MW38 = m.Var(lb=0.00,ub=596.40)
MW39 = m.Var(lb=0.00,ub=596.40)

MW40 = m.Var(lb=0.00,ub=456.79)
MW41 = m.Var(lb=0.00,ub=456.79)
MW42 = m.Var(lb=0.00,ub=456.79)

MW43 = m.Var(lb=0.00,ub=73.41)
MW44 = m.Var(lb=0.00,ub=73.41)
MW45 = m.Var(lb=0.00,ub=73.41)

MW46 = m.Var(lb=474.83,ub=593.54)
MW47 = m.Var(lb=477.12,ub=596.40)
MW48 = m.Var(lb=365.43,ub=456.79)
MW49 = m.Var(lb=58.79,ub=73.41)

MW50 = m.Var(lb=0.00,ub=593.54)
MW51 = m.Var(lb=0.00,ub=596.40)
MW52 = m.Var(lb=0.00,ub=456.79)
MW53 = m.Var(lb=0.00,ub=73.41)

MW54 = m.Var(lb=0.00,ub=593.54)
MW55 = m.Var(lb=0.00,ub=593.54)
MW56 = m.Var(lb=0.00,ub=593.54)
MW57 = m.Var(lb=0.00,ub=593.54)
MW58 = m.Var(lb=0.00,ub=593.54)
MW59 = m.Var(lb=0.00,ub=593.54)
MW60 = m.Var(lb=0.00,ub=593.54)

MW61 = m.Var(lb=0.00,ub=596.40)
MW62 = m.Var(lb=0.00,ub=596.40)
MW63 = m.Var(lb=0.00,ub=596.40)
MW64 = m.Var(lb=0.00,ub=596.40)
MW65 = m.Var(lb=0.00,ub=596.40)
MW66 = m.Var(lb=0.00,ub=596.40)
MW67 = m.Var(lb=0.00,ub=596.40)

MW68 = m.Var(lb=0.00,ub=456.79)
MW69 = m.Var(lb=0.00,ub=456.79)
MW70 = m.Var(lb=0.00,ub=456.79)
MW71 = m.Var(lb=0.00,ub=456.79)
MW72 = m.Var(lb=0.00,ub=456.79)
MW73 = m.Var(lb=0.00,ub=456.79)
MW74 = m.Var(lb=0.00,ub=456.79)

MW75 = m.Var(lb=0.00,ub=73.41)
MW76 = m.Var(lb=0.00,ub=73.41)
MW77 = m.Var(lb=0.00,ub=73.41)
MW78 = m.Var(lb=0.00,ub=73.41)
MW79 = m.Var(lb=0.00,ub=73.41)
MW80 = m.Var(lb=0.00,ub=73.41)
MW81 = m.Var(lb=0.00,ub=73.41)

MW82 = m.Var(lb=0.00,ub=593.54)
MW83 = m.Var(lb=0.00,ub=596.40)
MW84 = m.Var(lb=0.00,ub=456.79)
MW85 = m.Var(lb=0.00,ub=73.41)

MW86 = m.Var(lb=0.00,ub=1719.73)
MW87 = m.Var(lb=0.00,ub=1719.73)


MW87MED1 = m.Var(lb=0.00,ub=1719.73)
MW87MED2 = m.Var(lb=0.00,ub=1719.73)
MW87MED3 = m.Var(lb=0.00,ub=1719.73)
```

```
MW87MED4 = m.Var(lb=0.00,ub=1719.73)
MW87MED5 = m.Var(lb=0.00,ub=1719.73)




MFMED1 = m.Var(lb=0.00,ub=1719.73)
MFMED2 = m.Var(lb=0.00,ub=1719.73)
MFMED3 = m.Var(lb=0.00,ub=1719.73)
MFMED4 = m.Var(lb=0.00,ub=1719.73)
MFMED5 = m.Var(lb=0.00,ub=1719.73)





MW88 = m.Var(lb=0.00,ub=1719.73)



MW89 = m.Var(lb=0.00,ub=1719.73)
MW90 = m.Var(lb=0.00,ub=1719.73)
MW91 = m.Var(lb=0.00,ub=1719.73)
MW92 = m.Var(lb=0.00,ub=1719.73)
MW93 = m.Var(lb=0.00,ub=1719.73)
MW94 = m.Var(lb=0.00,ub=1719.73)
MW95 = m.Var(lb=0.00,ub=1719.73)
MW96 = m.Var(lb=0.00,ub=1719.73)
MW97A = m.Var(lb=0.00,ub=1719.73)


MW97 = m.Var(lb=0.00,ub=1719.73)
MW98 = m.Var(lb=0.00,ub=1719.73)
MW99 = m.Var(lb=0.00,ub=1719.73)

MW100 = m.Var(lb=0.00,ub=1719.73)
MW101 = m.Var(lb=0.00,ub=1719.73)
MW102 = m.Var(lb=0.00,ub=1719.73)
MW103 = m.Var(lb=0.00,ub=1719.73)
MW104 = m.Var(lb=0.00,ub=1719.73)

MW105 = m.Var(lb=0.00,ub=1719.73)





TW1 = 20.00

TW2 = 20.00
TW3 = 20.00
TW4 = 20.00
TW5 = 20.00



TW6 = 20.00
TW7 = 20.00
TW8 = 20.00
TW9 = 20.00
TW10 = 20.00

TW11 = 20.00
TW12 = 20.00
TW13 = 20.00
TW14 = 20.00
TW15 = 20.00

TW16 = 20.00
TW17 = 20.00
TW18 = 20.00
TW19 = 20.00
TW20 = 20.00

TW21 = 20.00
TW22 = 20.00
TW23 = 20.00
```

```
TW24 = 20.00
TW25 = 20.00

TW26 = m.Var(lb=20.00,ub=100.00)
TW27 = m.Var(lb=20.00,ub=100.00)
TW28 = m.Var(lb=20.00,ub=100.00)
TW29 = m.Var(lb=20.00,ub=100.00)

TW26A = m.Var(lb=20.00,ub=100.00)
TW27A = m.Var(lb=20.00,ub=100.00)
TW28A = m.Var(lb=20.00,ub=100.00)
TW29A = m.Var(lb=20.00,ub=100.00)

TW30 = m.Var(lb=20.00,ub=100.00)
TW31 = m.Var(lb=20.00,ub=100.00)
TW32 = m.Var(lb=20.00,ub=100.00)
TW33 = m.Var(lb=20.00,ub=100.00)

TW34 = m.Var(lb=20.00,ub=100.00)
TW35 = m.Var(lb=20.00,ub=100.00)
TW36 = m.Var(lb=20.00,ub=100.00)

TW37 = m.Var(lb=20.00,ub=100.00)
TW38 = m.Var(lb=20.00,ub=100.00)
TW39 = m.Var(lb=20.00,ub=100.00)

TW40 = m.Var(lb=20.00,ub=100.00)
TW41 = m.Var(lb=20.00,ub=100.00)
TW42 = m.Var(lb=20.00,ub=100.00)

TW43 = m.Var(lb=20.00,ub=100.00)
TW44 = m.Var(lb=20.00,ub=100.00)
TW45 = m.Var(lb=20.00,ub=100.00)

TW46 = 95.00
TW47 = 95.00
TW48 = 95.00
TW49 = 100.00

TW50 = 95.00
TW51 = 95.00
TW52 = 95.00
TW53 = 100.00

TW54 = 95.00
TW55 = 95.00
TW56 = 95.00
TW57 = 95.00
TW58 = 95.00
TW59 = 95.00
TW60 = 95.00

TW61 = 95.00
TW62 = 95.00
TW63 = 95.00
TW64 = 95.00
TW65 = 95.00
TW66 = 95.00
TW67 = 95.00

TW68 = 95.00
TW69 = 95.00
TW70 = 95.00
TW71 = 95.00
TW72 = 95.00
TW73 = 95.00
TW74 = 95.00

TW75 = 100.00
TW76 = 100.00
TW77 = 100.00
TW78 = 100.00
TW79 = 100.00
TW80 = 100.00
TW81 = 100.00

TW82 = m.Var(lb=20.00,ub=100.00)
```

```
TW83 = m.Var(lb=20.00,ub=100.00)
TW84 = m.Var(lb=20.00,ub=100.00)
TW85 = m.Var(lb=20.00,ub=100.00)

TW86 = m.Var(lb=20.00,ub=100.00)
TW87 = m.Var(lb=20.00,ub=100.00)


TW87MED = m.Var(lb=20.00,ub=100.00)





TW88 = 100.00

TW89 = 100.00
TW90 = 100.00
TW91 = 100.00
TW92 = 100.00
TW93 = 100.00
TW94 = 100.00
TW95 = 100.00
TW96 = 100.00
TW97A = 100.00
TW97B = 100.00

TW97 = m.Var(lb=20.00,ub=100.00)
TW98 = m.Var(lb=20.00,ub=100.00)
TW99 = m.Var(lb=20.00,ub=100.00)

TW100 = m.Var(lb=20.00,ub=100.00)
TW101 = m.Var(lb=20.00,ub=100.00)
TW102 = m.Var(lb=20.00,ub=100.00)
TW103 = m.Var(lb=20.00,ub=100.00)
TW104 = m.Var(lb=20.00,ub=100.00)

TW105 = 30.00






hW1 = 83.800

hW2 = 83.800
hW3 = 83.800
hW4 = 83.800
hW5 = 83.800



hW6 = 83.800
hW7 = 83.800
hW8 = 83.800
hW9 = 83.800
hW10 = 83.800

hW11 = 83.800
hW12 = 83.800
hW13 = 83.800
hW14 = 83.800
hW15 = 83.800

hW16 = 83.800
hW17 = 83.800
hW18 = 83.800
hW19 = 83.800
hW20 = 83.800

hW21 = 83.800
hW22 = 83.800
hW23 = 83.800
hW24 = 83.800
hW25 = 83.800
```

```
hW26 = m.Var(lb=83.800,ub=418.896)
hW27 = m.Var(lb=83.800,ub=418.896)
hW28 = m.Var(lb=83.800,ub=418.896)
hW29 = m.Var(lb=83.800,ub=418.896)

hW26A = m.Var(lb=83.800,ub=418.896)
hW27A = m.Var(lb=83.800,ub=418.896)
hW28A = m.Var(lb=83.800,ub=418.896)
hW29A = m.Var(lb=83.800,ub=418.896)

hW30 = m.Var(lb=83.800,ub=418.896)
hW31 = m.Var(lb=83.800,ub=418.896)
hW32 = m.Var(lb=83.800,ub=418.896)
hW33 = m.Var(lb=83.800,ub=418.896)

hW34 = m.Var(lb=83.800,ub=418.896)
hW35 = m.Var(lb=83.800,ub=418.896)
hW36 = m.Var(lb=83.800,ub=418.896)

hW37 = m.Var(lb=83.800,ub=418.896)
hW38 = m.Var(lb=83.800,ub=418.896)
hW39 = m.Var(lb=83.800,ub=418.896)

hW40 = m.Var(lb=83.800,ub=418.896)
hW41 = m.Var(lb=83.800,ub=418.896)
hW42 = m.Var(lb=83.800,ub=418.896)

hW43 = m.Var(lb=83.800,ub=418.896)
hW44 = m.Var(lb=83.800,ub=418.896)
hW45 = m.Var(lb=83.800,ub=418.896)

hW46 = 397.952
hW47 = 397.952
hW48 = 397.952
hW49 = 418.896

hW50 = 397.952
hW51 = 397.952
hW52 = 397.952
hW53 = 418.896

hW54 = 397.952
hW55 = 397.952
hW56 = 397.952
hW57 = 397.952
hW58 = 397.952
hW59 = 397.952
hW60 = 397.952

hW61 = 397.952
hW62 = 397.952
hW63 = 397.952
hW64 = 397.952
hW65 = 397.952
hW66 = 397.952
hW67 = 397.952

hW68 = 397.952
hW69 = 397.952
hW70 = 397.952
hW71 = 397.952
hW72 = 397.952
hW73 = 397.952
hW74 = 397.952

hW75 = 418.896
hW76 = 418.896
hW77 = 418.896
hW78 = 418.896
hW79 = 418.896
hW80 = 418.896
hW81 = 418.896

hW82 = m.Var(lb=83.800,ub=418.896)
hW83 = m.Var(lb=83.800,ub=418.896)
hW84 = m.Var(lb=83.800,ub=418.896)
hW85 = m.Var(lb=83.800,ub=418.896)
```

```
hW86 = m.Var(lb=83.800,ub=418.896)
hW87 = m.Var(lb=83.800,ub=418.896)


hW87MED = m.Var(lb=83.800,ub=418.896)


hW87MED1 = m.Var(lb=418.896,ub=2675.43)
hW87MED2 = m.Var(lb=418.896,ub=2675.43)
hW87MED3 = m.Var(lb=418.896,ub=2675.43)
hW87MED4 = m.Var(lb=418.896,ub=2675.43)
hW87MED5 = m.Var(lb=418.896,ub=2675.43)





hW88 = 418.896

hW89 = 418.896
hW90 = 418.896
hW91 = 418.896
hW92 = 418.896
hW93 = 418.896
hW94 = 418.896
hW95 = 418.896
hW96 = 418.896
hW97A = 418.896


hW97 = m.Var(lb=83.800,ub=418.896)
hW98 = m.Var(lb=83.800,ub=418.896)
hW99 = m.Var(lb=83.800,ub=418.896)

hW100 = m.Var(lb=83.800,ub=418.896)
hW101 = m.Var(lb=83.800,ub=418.896)
hW102 = m.Var(lb=83.800,ub=418.896)
hW103 = m.Var(lb=83.800,ub=418.896)
hW104 = m.Var(lb=83.800,ub=418.896)

hW105 = 125.687





CW1 = 0.00

CW2 = 0.00
CW3 = 0.00
CW4 = 0.00
CW5 = 0.00


CW6 = 0.00
CW7 = 0.00
CW8 = 0.00
CW9 = 0.00
CW10 = 0.00

CW11 = 0.00
CW12 = 0.00
CW13 = 0.00
CW14 = 0.00
CW15 = 0.00

CW16 = 0.00
CW17 = 0.00
CW18 = 0.00
CW19 = 0.00
CW20 = 0.00

CW21 = 0.00
CW22 = 0.00
CW23 = 0.00
```

```
CW24 = 0.00
CW25 = 0.00

CW26 = m.Var(lb=0.00,ub=2000.00)
CW27 = m.Var(lb=0.00,ub=2000.00)
CW28 = m.Var(lb=0.00,ub=2000.00)
CW29 = m.Var(lb=0.00,ub=2000.00)



CW46 = m.Var(lb=0.00,ub=200.00)
CW47 = m.Var(lb=0.00,ub=200.00)
CW48 = m.Var(lb=0.00,ub=200.00)
CW49 = m.Var(lb=0.00,ub=200.00)

CW50 = m.Var(lb=800.00,ub=1000.00)
CW51 = m.Var(lb=800.00,ub=1000.00)
CW52 = m.Var(lb=800.00,ub=1000.00)
CW53 = m.Var(lb=800.00,ub=1000.00)



CW82 = m.Var(lb=0.00,ub=2000.00)
CW83 = m.Var(lb=0.00,ub=2000.00)
CW84 = m.Var(lb=0.00,ub=2000.00)
CW85 = m.Var(lb=0.00,ub=2000.00)

CW86 = m.Var(lb=0.00,ub=2000.00)
CW87 = m.Var(lb=0.00,ub=2000.00)
CW88 = 0.00


CF1 = m.Var(lb=0.00)



CW97 = m.Var(lb=0.00,ub=2000.00)
CW98 = m.Var(lb=0.00,ub=2000.00)


CW105 = 0.00






q1 = m.Var(lb=0.00)
q2 = m.Var(lb=0.00)
q3 = m.Var(lb=0.00)
q4 = m.Var(lb=0.00)





qc = m.Var(lb=0.00)








## Additional Fuel System


MF1 = m.Var(lb=0.00,ub=1719.73)
MF2 = m.Var(lb=0.00,ub=1719.73)
MF2A1 = m.Var(lb=0.00,ub=1719.73)
MF2A2 = m.Var(lb=0.00,ub=1719.73)


AF1 = m.Var(lb=82.87022901)
AF2 = m.Var(lb=138.6570048)
```

```
LHV1 = m.Var(lb=0.0451e6,ub=0.12021e6)
LHV2 = m.Var(lb=0.0451e6,ub=0.12021e6)


XH2 = m.Var(lb=0.00,ub=1.00)



Y1 = m.Var(lb=0.00,ub=1.00)
Y2 = m.Var(lb=0.00,ub=1.00)



## Post-processing Purposes


M0 = m.Var(lb=0.00,ub=300.00)
q0 = m.Var(lb=0.00)


ORCEff = 6.00



# Constraints


## Thermal Process System


m.Equation(M2 + M4 + M12 == MA2)
m.Equation(M2 * h2 + M4 * h4 + M12 * h12 == MA2 * hA2)



m.Equation(M1 + MA2 == M7)
m.Equation(M1 * (h1 + LHV1) + MA2 * hA2 - (16480.50 * 1.05 * (548.4138253 - 230.00)) ==
M7 * h7)
m.Equation(M1 * AF1 == MA2)
m.Equation(M1 * LHV1 + MA2 * (hA2 - 302.595) == 9.255e6)




m.Equation(M3 == M4 + M5 + M6)
m.Equation(M3 * h3 == M4 * h4 + M5 * h5 + M6 * h6)



m.Equation(M9 + M11 + M5 == MA9)
m.Equation(M9 * h9 + M11 * h11 + M5 * h5 == MA9 * hA9)




m.Equation(M8 + MA9 == M14)
m.Equation(M8 * (h8 + LHV2) + MA9 * hA9 - 14454.50 * 1.05 * (350.3098849 - 159.30) ==
M14 * h14)
m.Equation(M8 * AF2 == MA9)
m.Equation(M8 * LHV2 + MA9 * (hA9 - 302.595) == 4.87485e6)




m.Equation(M10 == M11 + M12 + M13)
m.Equation(M10 * h10 == M11 * h11 + M12 * h12 + M13 * h13)




m.Equation(M6 + M13 == M15)
m.Equation(M6 * h6 + M13 * h13 == M15 * h15)
```

```
m.Equation(M7 + M14 == M16)
m.Equation(M7 * h7 + M14 * h14 == M16 * h16)



m.Equation(M15 == M15A1 + M15A2 + M15A3 + M15A4 + M15MED)


m.Equation(M15A1 * (h15 - h15A1) == qH1)

m.Equation(M15A2 * (h15 - h15A2) == qH2)

m.Equation(M15A3 * (h15 - h15A3) == qH3)

m.Equation(M15A4 * (h15 - h15A4) == qH4)

m.Equation(M15MED * (h15 - h15MED) == qMED)


m.Equation(M15A1 + M15A2 + M15A3 + M15A4 + M15MED + M16 == MORC)
m.Equation(M15A1 * h15A1 + M15A2 * h15A2 + M15A3 * h15A3 + M15A4 * h15A4 + M15MED *
h15MED + M16 * h16 == MORC * hORC)



m.Equation(MORC * (hORC - hORCOut) * (ORCEff * 0.01) == E * 3600)


m.Equation(E == E1 + E2 + EMED)




m.Equation(h7 == 1.0700 * T7 + 265.1454)
m.Equation(h14 == 1.0700 * T14 + 265.1454)
m.Equation(h15 == 1.0700 * T15 + 265.1454)
m.Equation(h16 == 1.0700 * T16 + 265.1454)
m.Equation(hA2 == 1.0700 * TA2 + 265.1454)
m.Equation(hA9 == 1.0700 * TA9 + 265.1454)



m.Equation(h15A1 == 1.0700 * T15A1 + 265.1454)
m.Equation(h15A2 == 1.0700 * T15A2 + 265.1454)
m.Equation(h15A3 == 1.0700 * T15A3 + 265.1454)
m.Equation(h15A4 == 1.0700 * T15A4 + 265.1454)
m.Equation(h15MED == 1.0700 * T15MED + 265.1454)
m.Equation(h15MEDInt == 1.0700 * T15MEDInt + 265.1454)



m.Equation(hORC == 1.0700 * TORC + 265.1454)
m.Equation(hORCOut == 1.0700 * TORCOut + 265.1454)




## Water System



m.Equation(MW1 == MW2 + MW3 + MW4 + MW5)




m.Equation(MW2 == MW6 + MW7 + MW8 + MW9 + MW10)
```

```
m.Equation(MW3 == MW11 + MW12 + MW13 + MW14 + MW15)





m.Equation(MW4 == MW16 + MW17 + MW18 + MW19 + MW20)





m.Equation(MW5 == MW21 + MW22 + MW23 + MW24 + MW25)






m.Equation(MW6 + (MW55 + MW62 + MW69 + MW76) + (MW90) + MW100 == MW26)
m.Equation(MW6 * hW6 + (MW55 * hW55 + MW62 * hW62 + MW69 * hW69 + MW76 * hW76) + (MW90
* hW90) + MW100 * hW98 == MW26 * hW26)
m.Equation(MW6 * CW6 + (MW55 * CW50 + MW62 * CW51 + MW69 * CW52 + MW76 * CW53) + (MW90
* CW88) + MW100 * CW98 == MW26 * CW26)

m.Equation(MW11 + (MW56 + MW63 + MW70 + MW77) + (MW91) + MW101 == MW27)
m.Equation(MW11 * hW11 + (MW56 * hW56 + MW63 * hW63 + MW70 * hW70 + MW77 * hW77) +
(MW91 * hW91) + MW101 * hW98 == MW27 * hW27)
m.Equation(MW11 * CW11 + (MW56 * CW50 + MW63 * CW51 + MW70 * CW52 + MW77 * CW53) +
(MW91 * CW88) + MW101 * CW98 == MW27 * CW27)

m.Equation(MW16 + (MW57 + MW64 + MW71 + MW78) + (MW92) + MW102 == MW28)
m.Equation(MW16 * hW16 + (MW57 * hW57 + MW64 * hW64 + MW71 * hW71 + MW78 * hW78) +
(MW92 * hW92) + MW102 * hW98 == MW28 * hW28)
m.Equation(MW16 * CW16 + (MW57 * CW50 + MW64 * CW51 + MW71 * CW52 + MW78 * CW53) +
(MW92 * CW88) + MW101 * CW98 == MW28 * CW28)

m.Equation(MW21 + (MW58 + MW65 + MW72 + MW79) + (MW93) + MW103 == MW29)
m.Equation(MW21 * hW21 + (MW58 * hW58 + MW65 * hW65 + MW72 * hW72 + MW79 * hW79) +
(MW93 * hW93) + MW103 * hW98 == MW29 * hW29)
m.Equation(MW21 * CW21 + (MW58 * CW50 + MW65 * CW51 + MW72 * CW52 + MW79 * CW53) +
(MW93 * CW88) + MW103 * CW98 == MW29 * CW29)






m.Equation(MW26 == MW26A)
m.Equation(MW26 * hW26 + qH1 == MW26A * hW26A)
m.Equation(qH1 * (1000 / 3600) == 400 * AH1 * (((T15 - TW26A) * (T15A1 - TW26) * ((T15
- TW26A) + (T15A1 - TW26)) * 0.5) ** (1 / 3)))

m.Equation(MW26A == MW30)
m.Equation(MW26A * hW26A + 0.850 * q1 == MW30 * hW30)
m.Equation(MW26A * CW26 == MW30 * CW26)



m.Equation(MW27 == MW27A)
m.Equation(MW27 * hW27 + qH2 == MW27A * hW27A)
m.Equation(qH2 * (1000 / 3600) == 400 * AH2 * (((T15 - TW27A) * (T15A2 - TW27) * ((T15
- TW27A) + (T15A2 - TW27)) * 0.5) ** (1 / 3)))

m.Equation(MW27A == MW31)
m.Equation(MW27A * hW27A + 0.821 * q2 == MW31 * hW31)
m.Equation(MW27A * CW27 == MW31 * CW27)



m.Equation(MW28 == MW28A)
m.Equation(MW28 * hW28 + qH3 == MW28A * hW28A)
m.Equation(qH3 * (1000 / 3600) == 400 * AH3 * (((T15 - TW28A) * (T15A3 - TW28) * ((T15
- TW28A) + (T15A3 - TW28)) * 0.5) ** (1 / 3)))

m.Equation(MW28A == MW32)
m.Equation(MW28A * hW28A + 0.866 * q3 == MW32 * hW32)
```

```
m.Equation(MW28A * CW28 == MW32 * CW28)



m.Equation(MW29 == MW29A)
m.Equation(MW29 * hW29 + qH4 == MW29A * hW29A)
m.Equation(qH4 * (1000 / 3600) == 400 * AH4 * (((T15 - TW29A) * (T15A4 - TW29) * ((T15
- TW29A) + (T15A4 - TW29)) * 0.5) ** (1 / 3)))

m.Equation(MW29A == MW33)
m.Equation(MW29A * hW29A + 0.870 * q4 == MW33 * hW33)
m.Equation(MW29A * CW29 == MW33 * CW29)







m.Equation(MW30 == MW34 + MW35 + MW36)
m.Equation(hW30 == hW34)
m.Equation(hW30 == hW35)
m.Equation(hW30 == hW36)


m.Equation(MW31 == MW37 + MW38 + MW39)
m.Equation(hW31 == hW37)
m.Equation(hW31 == hW38)
m.Equation(hW31 == hW39)


m.Equation(MW32 == MW40 + MW41 + MW42)
m.Equation(hW32 == hW40)
m.Equation(hW32 == hW41)
m.Equation(hW32 == hW42)


m.Equation(MW33 == MW43 + MW44 + MW45)
m.Equation(hW33 == hW43)
m.Equation(hW33 == hW44)
m.Equation(hW33 == hW45)




m.Equation(MW34 + MW94 + MW7 == MW46)
m.Equation(MW34 * hW34 + MW94 * hW94 + MW7 * hW7 == MW46 * hW46)
m.Equation(MW34 * CW26 + MW94 * CW88 + MW7 * CW7 == MW46 * CW46)

m.Equation(MW37 + MW95 + MW12 == MW47)
m.Equation(MW37 * hW37 + MW95 * hW95 + MW12 * hW12 == MW47 * hW47)
m.Equation(MW37 * CW27 + MW95 * CW88 + MW12 * CW12 == MW47 * CW47)

m.Equation(MW40 + MW96 + MW17 == MW48)
m.Equation(MW40 * hW40 + MW96 * hW96 + MW17 * hW17 == MW48 * hW48)
m.Equation(MW40 * CW28 + MW96 * CW88 + MW17 * CW17 == MW48 * CW48)

m.Equation(MW43 + MW97A + MW22 == MW49)
m.Equation(MW43 * hW43 + MW97A * hW97A + MW22 * hW22 == MW49 * hW49)
m.Equation(MW43 * CW29 + MW97A * CW88 + MW22 * CW22 == MW49 * CW49)



m.Equation(MW46 == MW50)
m.Equation(MW46 * (CW46 * (10**-6)) + 0.47483 == MW50 * (CW50 * (10**-6)))


m.Equation(MW47 == MW51)
m.Equation(MW47 * (CW47 * (10**-6)) + 0.47712 == MW51 * (CW51 * (10**-6)))


m.Equation(MW48 == MW52)
m.Equation(MW48 * (CW48 * (10**-6)) + 0.36543 == MW52 * (CW52 * (10**-6)))


m.Equation(MW49 == MW53)
m.Equation(MW49 * (CW49 * (10**-6)) + 0.05873 == MW53 * (CW53 * (10**-6)))
```

```
m.Equation(MW50 == MW54 + MW55 + MW56 + MW57 + MW58 + MW59 + MW60)
m.Equation(MW50 * hW50 == MW54 * hW54 + MW55 * hW55 + MW56 * hW56 + MW57 * hW57 + MW58
* hW58 + MW59 * hW59 + MW60 * hW60)


m.Equation(MW51 == MW61 + MW62 + MW63 + MW64 + MW65 + MW66 + MW67)
m.Equation(MW51 * hW51 == MW61 * hW61 + MW62 * hW62 + MW63 * hW63 + MW64 * hW64 + MW65
* hW65 + MW66 * hW66 + MW67 * hW67)


m.Equation(MW52 == MW68 + MW69 + MW70 + MW71 + MW72 + MW73 + MW74)
m.Equation(MW52 * hW52 == MW68 * hW68 + MW69 * hW69 + MW70 * hW70 + MW71 * hW71 + MW72
* hW72 + MW73 * hW73 + MW74 * hW74)


m.Equation(MW53 == MW75 + MW76 + MW77 + MW78 + MW79 + MW80 + MW81)
m.Equation(MW53 * hW53 == MW75 * hW75 + MW76 * hW76 + MW77 * hW77 + MW78 * hW78 + MW79
* hW79 + MW80 * hW80 + MW81 * hW81)




m.Equation(MW54 + MW8 == MW82)
m.Equation(MW54 * hW54 + MW8 * hW8 == MW82 * hW82)
m.Equation(MW54 * CW50 + MW8 * CW8 + MW35 * CW26 == MW82 * CW82)

m.Equation(MW61 + MW13 == MW83)
m.Equation(MW61 * hW61 + MW13 * hW13 == MW83 * hW83)
m.Equation(MW61 * CW51 + MW13 * CW13 == MW83 * CW83)

m.Equation(MW68 + MW18 == MW84)
m.Equation(MW68 * hW68 + MW18 * hW18 == MW84 * hW84)
m.Equation(MW68 * CW52 + MW18 * CW18 == MW84 * CW84)

m.Equation(MW75 + MW23 == MW85)
m.Equation(MW75 * hW75 + MW23 * hW23 == MW85 * hW85)
m.Equation(MW75 * CW53 + MW23 * CW23 == MW85 * CW85)



m.Equation(MW82 + MW83 + MW84 + MW85 == MW86)
m.Equation(MW82 * hW82 + MW83 * hW83 + MW84 * hW84 + MW85 * hW85 == MW86 * hW86)
m.Equation(MW82 * CW82 + MW83 * CW83 + MW84 * CW84 + MW85 * CW85 == MW86 * CW86)



m.Equation(MW86 + (MW35 + MW38 + MW41 + MW42) + MW104 == MW87)
m.Equation(MW86 * hW86 + (MW35 * hW35 + MW38 * hW38 + MW41 * hW41 + MW42 * hW42) +
MW104 * hW104 == MW87 * hW87)
m.Equation(MW86 * CW86 + (MW35 * CW26 + MW38 * CW27 + MW41 * CW28 + MW42 * CW28) +
MW104 * CW98 == MW87 * CW87)






m.Equation(MW87 * (hW87MED - hW87) + qMEDLoss == MW87MED5 * (hW87MED5 - 418.896))


m.Equation(MW87 * (1 / 5) == MW87MED1 + MFMED1)
m.Equation(qMED == MW87MED1 * (hW87MED1 - 418.896) + MW87 * (1 / 5) * (418.896 -
hW87MED))
m.Equation(MW87MED1 * (2675.43 - 418.896) == MW87 * (1 / 5) * (hW87MED1 - 418.896))



m.Equation(MW87MED1 * (hW87MED1 - 418.896)  * (1000 / 3600) == 400 * AHMED * (((T15 -
100.00) * (T15MEDInt - 100.00) * (((T15 - 100.00) + (T15MEDInt - 100.00)) * 0.5)) ** (1
/ 3)))
```

```
m.Equation(MW87 * (1 / 5) * (418.896 - hW87MED) == M15MED * (h15MEDInt - h15MED))



m.Equation(MW87 * (1 / 5) == MW87MED2 + MFMED2)
m.Equation(MW87MED1 * (hW87MED1 - 418.896) == MW87MED2 * (hW87MED2 - 418.896) + MW87 *
(1 / 5) * (418.896 - hW87MED))
m.Equation(MW87MED2 * (2675.43 - 418.896) == MW87 * (1 / 5) * (hW87MED2 - 418.896))


m.Equation(MW87 * (1 / 5) == MW87MED3 + MFMED3)
m.Equation(MW87MED2 * (hW87MED2 - 418.896) == MW87MED3 * (hW87MED3 - 418.896) + MW87 *
(1 / 5) * (418.896 - hW87MED))
m.Equation(MW87MED3 * (2675.43 - 418.896) == MW87 * (1 / 5) * (hW87MED3 - 418.896))


m.Equation(MW87 * (1 / 5) == MW87MED4 + MFMED4)
m.Equation(MW87MED3 * (hW87MED3 - 418.896) == MW87MED4 * (hW87MED4 - 418.896) + MW87 *
(1 / 5) * (418.896 - hW87MED))
m.Equation(MW87MED4 * (2675.43 - 418.896) == MW87 * (1 / 5) * (hW87MED4 - 418.896))


m.Equation(MW87 * (1 / 5) == MW87MED5 + MFMED5)
m.Equation(MW87MED4 * (hW87MED4 - 418.896) == MW87MED5 * (hW87MED5 - 418.896) + MW87 *
(1 / 5) * (418.896 - hW87MED))
m.Equation(MW87MED5 * (2675.43 - 418.896) == MW87 * (1 / 5) * (hW87MED5 - 418.896))




m.Equation(MW87MED1 + MW87MED2 + MW87MED3 + MW87MED4 + MW87MED5 == MW88)



m.Equation(MW87 == MW88 + MF1)

m.Equation(MW87 * CW87 == MW88 * CW88 + MF1 * CF1)


m.Equation(EMED == 2.5 * (MW88 / 999))








m.Equation(MW88 == MW89 + MW90 + MW91 + MW92 + MW93 + MW94 + MW95 + MW96 + MW97A)
m.Equation(MW88 * hW88 == MW89 * hW89 + MW90 * hW90 + MW91 * hW91 + MW92 * hW92 + MW93
* hW93 + MW94 * hW94 + MW95 * hW95 + MW96 * hW96 + MW97A * hW97A)



m.Equation(MW89 + (MW10 + MW15 + MW20 + MW25) + (MW59 + MW66 + MW73 + MW80) == MW97)
m.Equation(MW89 * hW89 + (MW10 * hW10 + MW15 * hW15 + MW20 * hW20 + MW25 * hW25) +
(MW59 * hW59 + MW66 * hW66 + MW73 * hW73 + MW80 * hW80) == MW97 * hW97)
m.Equation(MW89 * CW88 + (MW10 * CW10 + MW15 * CW15 + MW20 * CW20 + MW25 * CW25) +
(MW59 * CW50 + MW66 * hW66 + MW73 * CW52 + MW80 * CW53) == MW97 * CW97)



m.Equation(MW97 == MW98)
m.Equation(MW97 * hW97 == MW98 * hW98 + qc)
m.Equation(MW97 * CW97 == MW98 * CW98)



m.Equation(MW98 == MW99 + MW100 + MW101 + MW102 + MW103 + MW104)
m.Equation(MW98 * hW98 == MW99 * hW99 + MW100 * hW100 + MW101 * hW101 + MW102 * hW102 +
MW103 * hW103 + MW104 * hW104)
m.Equation(hW98 == hW99)
m.Equation(hW98 == hW100)
m.Equation(hW98 == hW101)
m.Equation(hW98 == hW102)
```

```
m.Equation(hW98 == hW103)
m.Equation(hW98 == hW104)



m.Equation(MW99 + (MW9 + MW14 + MW19 + MW24) + (MW36 + MW39 + MW42 + MW45) + (MW60 +
MW67 + MW74 + MW81) == MW105)
m.Equation(MW99 * hW99 + (MW9 * hW9 + MW14 * hW14 + MW19 * hW19 + MW24 * hW24) + (MW36
* hW36 + MW39 * hW39 + MW42 * hW42 + MW45 * hW45) + (MW60 * hW60 + MW67 * hW67 + MW74 *
hW74 + MW81 * hW81) == MW105 * hW105)
m.Equation(MW99 * CW98 + (MW9 * CW9 + MW14 * CW14 + MW19 * CW19 + MW24 * CW24) + (MW36
* CW26 + MW39 * CW27 + MW42 * CW28 + MW45 * CW29) + (MW60 * CW50 + MW67 * CW51 + MW74 *
CW52 + MW81 * CW53)  == MW105 * CW105)







m.Equation(hW26 == 4.1887 * TW26 + 0.0259)
m.Equation(hW27 == 4.1887 * TW27 + 0.0259)
m.Equation(hW28 == 4.1887 * TW28 + 0.0259)
m.Equation(hW29 == 4.1887 * TW29 + 0.0259)

m.Equation(hW26A == 4.1887 * TW26A + 0.0259)
m.Equation(hW27A == 4.1887 * TW27A + 0.0259)
m.Equation(hW28A == 4.1887 * TW28A + 0.0259)
m.Equation(hW29A == 4.1887 * TW29A + 0.0259)



m.Equation(hW30 == 4.1887 * TW30 + 0.0259)
m.Equation(hW31 == 4.1887 * TW31 + 0.0259)
m.Equation(hW32 == 4.1887 * TW32 + 0.0259)
m.Equation(hW33 == 4.1887 * TW33 + 0.0259)
m.Equation(hW34 == 4.1887 * TW34 + 0.0259)
m.Equation(hW35 == 4.1887 * TW35 + 0.0259)
m.Equation(hW36 == 4.1887 * TW36 + 0.0259)
m.Equation(hW37 == 4.1887 * TW37 + 0.0259)
m.Equation(hW38 == 4.1887 * TW38 + 0.0259)
m.Equation(hW39 == 4.1887 * TW39 + 0.0259)
m.Equation(hW40 == 4.1887 * TW40 + 0.0259)
m.Equation(hW41 == 4.1887 * TW41 + 0.0259)
m.Equation(hW42 == 4.1887 * TW42 + 0.0259)
m.Equation(hW43 == 4.1887 * TW43 + 0.0259)
m.Equation(hW44 == 4.1887 * TW44 + 0.0259)
m.Equation(hW45 == 4.1887 * TW45 + 0.0259)




m.Equation(hW82 == 4.1887 * TW82 + 0.0259)
m.Equation(hW83 == 4.1887 * TW83 + 0.0259)
m.Equation(hW84 == 4.1887 * TW84 + 0.0259)
m.Equation(hW85 == 4.1887 * TW85 + 0.0259)
m.Equation(hW86 == 4.1887 * TW86 + 0.0259)
m.Equation(hW87 == 4.1887 * TW87 + 0.0259)
m.Equation(hW87MED == 4.1887 * TW87MED + 0.0259)



m.Equation(hW97 == 4.1887 * TW97 + 0.0259)
m.Equation(hW98 == 4.1887 * TW98 + 0.0259)
m.Equation(hW99 == 4.1887 * TW99 + 0.0259)
m.Equation(hW100 == 4.1887 * TW100 + 0.0259)
m.Equation(hW101 == 4.1887 * TW101 + 0.0259)
m.Equation(hW102 == 4.1887 * TW102 + 0.0259)
m.Equation(hW103 == 4.1887 * TW103 + 0.0259)
m.Equation(hW104 == 4.1887 * TW104 + 0.0259)



## Additional Fuel System


m.Equation(((MW105) / 0.01801528) * XH2 == (MF2 / 0.002016))
```

```
m.Equation(((MW105) / 0.01801528) * 285.85 * XH2 == 0.7 * (E1 * 3600))

m.Equation(MF2 == MF2A1 + MF2A2)




m.Equation(MF2A1 + M1Z == M1)
m.Equation(MF2A1 * (0.12021E6) + M1Z * (0.0451E6) == M1 * LHV1)
m.Equation(AF1 == (LHV1 / (0.0451E6)) * 82.87022901)



m.Equation(MF2A2 + M2Z == M8)
m.Equation(MF2A2 * (0.12021E6) + M2Z * (0.0451E6) == M8 * LHV2)
m.Equation(AF2 == (LHV2 / (0.0451E6)) * 138.6570048)


m.Equation(MW1 == MW105 + MF1)
m.Equation(0.47483 + 0.47712 + 0.36543 + 0.05873 == MW105 * ((CW105 * (10**-6))) + MF1
* ((CF1 * (10**-6))))
m.Equation(MW1 * hW1 + q1 + q2 + q3 + q4 + qH1 + qH2 + qH3 + qH4 + qMED == MW105 *
hW105 + MF1 * 418.896 + qMEDLoss + qc)



m.Equation(((MF2A1 / 0.002016) + (M1Z / 0.01900)) * Y1 == MF2A1 / 0.002016)
m.Equation(((MF2A2 / 0.002016) + (M2Z / 0.01900)) * Y2 == MF2A2 / 0.002016)



## Post-processing Purposes



m.Equation(M0 == M1Z + M2Z)
m.Equation(q0 == q1 + q2 + q3 + q4)





# Objective-Function (Minimization of Total Annualized Costs)

m.Obj(23.66 * 0.0451 * M0 + 1.8499 * (MW1 / 999) + (23.66e-6) * q0 + 0.1459 * (1 /
0.95) * (1 / 3600) * qc + 0.1459 * (-E2)) # Objective


m.solve() # Solve
```

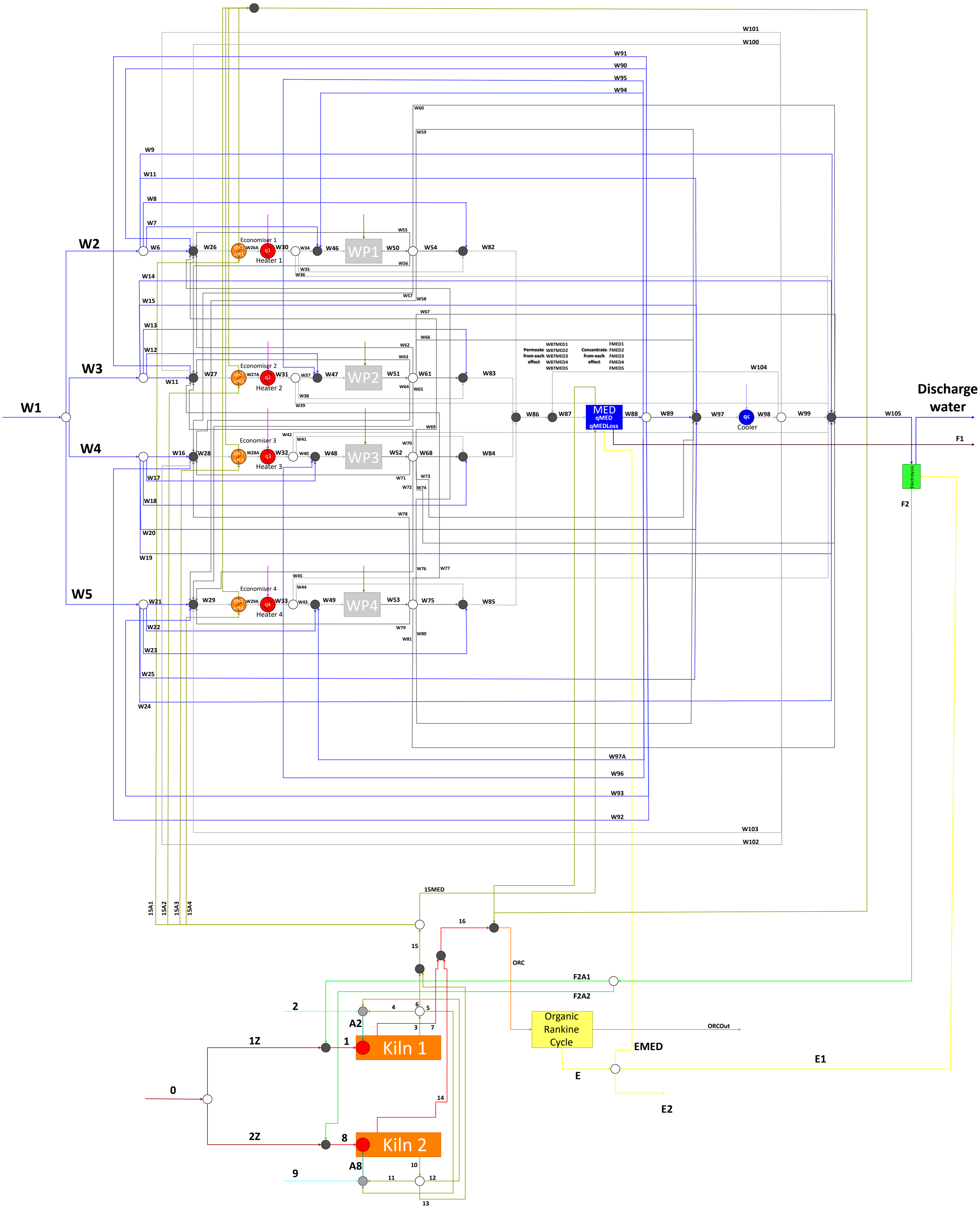


Figure A5. Flowsheet for the Case-study 1 WEIS including the stream and sizing parameters references considered in the scripting of the optimisation model Python code

A6. Case-study 2 Optimisation Model for the Water System (Python code)

The NLP model developed for the water system of case-study 2 is presented in Code Listing A2. The association of the defined variables to each stream and WEIS component for case-study 2 is presented in the further appendix (in which each stream/ component within the WEIS flow sheet is characterized according to its definition in the developed code).

Code Listing A2. Optimisation model for the water system of Case-study 2 (Python code)

```
from gekko import GEKKO



# CS1 Model Setup

m = GEKKO() # Initialization
m.options.SOLVER=3 # Definition of IPOPT solver



# Setup of APOPT Solver
m.solver_options = ['max_iter 500000',
                    'linear_solver mumps',\
                    'mu_strategy adaptive']



# Decision Variables





## Water System



MW1     = m.Var(lb=0.00,ub=1031.63)

MW2     = m.Var(lb=0.00,ub=373.68)
MW3     = m.Var(lb=0.00,ub=583.13)
MW3A    = m.Var(lb=0.00,ub=74.82)

MW4     = m.Var(lb=0.00,ub=373.68)
MW5     = m.Var(lb=0.00,ub=373.68)
MW6     = m.Var(lb=0.00,ub=373.68)
MW7     = m.Var(lb=0.00,ub=373.68)
MW8     = m.Var(lb=0.00,ub=373.68)

MW9     = m.Var(lb=0.00,ub=583.13)
MW10    = m.Var(lb=0.00,ub=583.13)
MW11    = m.Var(lb=0.00,ub=583.13)
MW12    = m.Var(lb=0.00,ub=583.13)
MW13    = m.Var(lb=0.00,ub=583.13)

MW14    = m.Var(lb=0.00,ub=74.82)
MW15    = m.Var(lb=0.00,ub=74.82)
MW16    = m.Var(lb=0.00,ub=74.82)
MW17    = m.Var(lb=0.00,ub=74.82)
MW18    = m.Var(lb=0.00,ub=74.82)

MW19    = m.Var(lb=0.00,ub=373.68)
MW20    = m.Var(lb=0.00,ub=583.13)
MW21    = m.Var(lb=0.00,ub=74.82)

MW22    = m.Var(lb=0.00,ub=373.68)
MW23    = m.Var(lb=0.00,ub=583.13)
MW24    = m.Var(lb=0.00,ub=74.82)
```

```
MW25     = m.Var(lb=0.00,ub=373.68)
MW26     = m.Var(lb=0.00,ub=373.68)
MW27     = m.Var(lb=0.00,ub=373.68)

MW28    = m.Var(lb=0.00,ub=583.13)
MW29    = m.Var(lb=0.00,ub=583.13)
MW30    = m.Var(lb=0.00,ub=583.13)

MW31    = m.Var(lb=0.00,ub=74.82)
MW32    = m.Var(lb=0.00,ub=74.82)
MW33    = m.Var(lb=0.00,ub=74.82)

MW34    = m.Var(lb=0.00,ub=373.68)
MW35    = m.Var(lb=0.00,ub=583.13)
MW36    = m.Var(lb=0.00,ub=74.82)

MW37    = m.Var(lb=0.00,ub=373.68)
MW38    = m.Var(lb=0.00,ub=583.13)
MW39    = m.Var(lb=0.00,ub=74.82)

MW40    = m.Var(lb=0.00,ub=373.68)
MW41    = m.Var(lb=0.00,ub=373.68)
MW42    = m.Var(lb=0.00,ub=373.68)
MW43    = m.Var(lb=0.00,ub=373.68)
MW44    = m.Var(lb=0.00,ub=373.68)
MW45    = m.Var(lb=0.00,ub=373.68)
MW46    = m.Var(lb=0.00,ub=373.68)
MW47    = m.Var(lb=0.00,ub=373.68)

MW48    = m.Var(lb=0.00,ub=583.13)
MW49    = m.Var(lb=0.00,ub=583.13)
MW50    = m.Var(lb=0.00,ub=583.13)
MW51    = m.Var(lb=0.00,ub=583.13)
MW52    = m.Var(lb=0.00,ub=583.13)
MW53    = m.Var(lb=0.00,ub=583.13)
MW54    = m.Var(lb=0.00,ub=583.13)
MW55    = m.Var(lb=0.00,ub=583.13)

MW56    = m.Var(lb=0.00,ub=74.82)
MW57    = m.Var(lb=0.00,ub=74.82)
MW58    = m.Var(lb=0.00,ub=74.82)
MW59    = m.Var(lb=0.00,ub=74.82)
MW60    = m.Var(lb=0.00,ub=74.82)
MW61    = m.Var(lb=0.00,ub=74.82)
MW62    = m.Var(lb=0.00,ub=74.82)
MW63    = m.Var(lb=0.00,ub=74.82)

MW64    = m.Var(lb=0.00,ub=373.68)
MW65    = m.Var(lb=0.00,ub=583.13)
MW66    = m.Var(lb=0.00,ub=74.82)



MW67    = m.Var(lb=0.00,ub=1031.63)
MW67MED = m.Var(lb=0.00,ub=1031.63)

MW67MEDV1 = m.Var(lb=0.00,ub=1031.63)
MWSludge= m.Var(lb=0.00,ub=1031.63)

MW67MEDV2 = m.Var(lb=0.00,ub=1031.63)
MWSludge2 = m.Var(lb=0.00,ub=1031.63)

MW67MEDV3 = m.Var(lb=0.00,ub=1031.63)
MWSludge3 = m.Var(lb=0.00,ub=1031.63)

MW67MEDV4 = m.Var(lb=0.00,ub=1031.63)
MWSludge4 = m.Var(lb=0.00,ub=1031.63)


MF1 = m.Var(lb=0.00,ub=1031.63)



MW68    = m.Var(lb=0.00,ub=1031.63)

MW69    = m.Var(lb=0.00,ub=1031.63)
MW70    = m.Var(lb=0.00,ub=1031.63)
```

```
MW71    = m.Var(lb=0.00,ub=1031.63)
MW72    = m.Var(lb=0.00,ub=1031.63)
MW73    = m.Var(lb=0.00,ub=1031.63)
MW74    = m.Var(lb=0.00,ub=1031.63)
MW75    = m.Var(lb=0.00,ub=1031.63)
MW76    = m.Var(lb=0.00,ub=1031.63)


MW79    = m.Var(lb=0.00,ub=373.68)
MW80    = m.Var(lb=0.00,ub=583.13)
MW81    = m.Var(lb=0.00,ub=74.82)

MW82    = m.Var(lb=0.00,ub=373.68)
MW83    = m.Var(lb=0.00,ub=583.13)
MW84    = m.Var(lb=0.00,ub=74.82)


MW85    = m.Var(lb=0.00,ub=373.68)
MW86    = m.Var(lb=0.00,ub=583.13)
MW87    = m.Var(lb=0.00,ub=74.82)

MW88    = m.Var(lb=0.00,ub=373.68)
MW89    = m.Var(lb=0.00,ub=373.68)
MW90    = m.Var(lb=0.00,ub=373.68)

MW91    = m.Var(lb=0.00,ub=583.13)
MW92    = m.Var(lb=0.00,ub=583.13)
MW93    = m.Var(lb=0.00,ub=583.13)

MW94    = m.Var(lb=0.00,ub=74.82)
MW95    = m.Var(lb=0.00,ub=74.82)
MW96    = m.Var(lb=0.00,ub=74.82)

MW97    = m.Var(lb=0.00,ub=1031.63)
MW98    = m.Var(lb=0.00,ub=1031.63)





TW1     = 20.00

TW2     = 20.00
TW3     = 20.00
TW3A    = 20.00

TW4     = 20.00
TW5     = 20.00
TW6     = 20.00
TW7     = 20.00
TW8     = 20.00

TW9     = 20.00
TW10    = 20.00
TW11    = 20.00
TW12    = 20.00
TW13    = 20.00

TW14    = 20.00
TW15    = 20.00
TW16    = 20.00
TW17    = 20.00
TW18    = 20.00

TW19    = m.Var(lb=20.00,ub=100.00)
TW20    = m.Var(lb=20.00,ub=100.00)
TW21    = m.Var(lb=20.00,ub=100.00)


TW19A   = m.Var(lb=20.00,ub=100.00)
TW20A   = m.Var(lb=20.00,ub=100.00)
TW21A   = m.Var(lb=20.00,ub=100.00)



TW22    = m.Var(lb=20.00,ub=100.00)
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```
TW23    = m.Var(lb=20.00,ub=100.00)
TW24    = m.Var(lb=20.00,ub=100.00)

TW25    = m.Var(lb=20.00,ub=100.00)
TW26    = m.Var(lb=20.00,ub=100.00)
TW27    = m.Var(lb=20.00,ub=100.00)

TW28    = m.Var(lb=20.00,ub=100.00)
TW29    = m.Var(lb=20.00,ub=100.00)
TW30    = m.Var(lb=20.00,ub=100.00)

TW31    = m.Var(lb=20.00,ub=100.00)
TW32    = m.Var(lb=20.00,ub=100.00)
TW33    = m.Var(lb=20.00,ub=100.00)

TW34    = 95.00
TW35    = 95.00
TW36    = 95.00




TW37    = 95.00
TW38    = 95.00
TW39    = 95.00

TW40    = 95.00
TW41    = 95.00
TW42    = 95.00
TW43    = 95.00
TW44    = 95.00
TW45    = 95.00
TW46    = 95.00
TW47    = 95.00

TW48    = 95.00
TW49    = 95.00
TW50    = 95.00
TW51    = 95.00
TW52    = 95.00
TW53    = 95.00
TW54    = 95.00
TW55    = 95.00

TW56    = 95.00
TW57    = 95.00
TW58    = 95.00
TW59    = 95.00
TW60    = 95.00
TW61    = 95.00
TW62    = 95.00
TW63    = 95.00

TW64    = m.Var(lb=20.00,ub=100.00)
TW65    = m.Var(lb=20.00,ub=100.00)
TW66    = m.Var(lb=20.00,ub=100.00)

TW67    = m.Var(lb=20.00,ub=100.00)
TW67MED = m.Var(lb=20.00,ub=100.00)

TW68    = 100.00

TW69    = 100.00
TW70    = 100.00
TW71    = 100.00
TW72    = 100.00
TW73    = 100.00
TW74    = 100.00
TW75    = 100.00
TW76    = 100.00


TW79    = 100.00
TW80    = 100.00
TW81    = 100.00

TW82    = m.Var(lb=33.00,ub=100.00)
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```
TW83    = m.Var(lb=33.00,ub=100.00)
TW84    = m.Var(lb=33.00,ub=100.00)


TW85    = m.Var(lb=33.00,ub=100.00)
TW86    = m.Var(lb=33.00,ub=100.00)
TW87    = m.Var(lb=33.00,ub=100.00)

TW88    = m.Var(lb=33.00,ub=100.00)
TW89    = m.Var(lb=33.00,ub=100.00)
TW90    = m.Var(lb=33.00,ub=100.00)

TW91    = m.Var(lb=33.00,ub=100.00)
TW92    = m.Var(lb=33.00,ub=100.00)
TW93    = m.Var(lb=33.00,ub=100.00)

TW94    = m.Var(lb=33.00,ub=100.00)
TW95    = m.Var(lb=33.00,ub=100.00)
TW96    = m.Var(lb=33.00,ub=100.00)

TW97    = m.Var(lb=33.00,ub=100.00)
TW98    = 33.33



hW1     = 83.799

hW2     = 83.799
hW3     = 83.799
hW3A    = 83.799

hW4     = 83.799
hW5     = 83.799
hW6     = 83.799
hW7     = 83.799
hW8     = 83.799

hW9     = 83.799
hW10    = 83.799
hW11    = 83.799
hW12    = 83.799
hW13    = 83.799

hW14    = 83.799
hW15    = 83.799
hW16    = 83.799
hW17    = 83.799
hW18    = 83.799

hW19    = m.Var(lb=83.799,ub=418.892)
hW20    = m.Var(lb=83.799,ub=418.892)
hW21    = m.Var(lb=83.799,ub=418.892)


hW19A   = m.Var(lb=83.799,ub=418.892)
hW20A   = m.Var(lb=83.799,ub=418.892)
hW21A   = m.Var(lb=83.799,ub=418.892)



hW22    = m.Var(lb=83.799,ub=418.892)
hW23    = m.Var(lb=83.799,ub=418.892)
hW24    = m.Var(lb=83.799,ub=418.892)

hW25    = m.Var(lb=83.799,ub=418.892)
hW26    = m.Var(lb=83.799,ub=418.892)
hW27    = m.Var(lb=83.799,ub=418.892)

hW28    = m.Var(lb=83.799,ub=418.892)
hW29    = m.Var(lb=83.799,ub=418.892)
hW30    = m.Var(lb=83.799,ub=418.892)

hW31    = m.Var(lb=83.799,ub=418.892)
hW32    = m.Var(lb=83.799,ub=418.892)
hW33    = m.Var(lb=83.799,ub=418.892)

hW34    = 397.949
```

```
hW35    = 397.949
hW36    = 397.949


hW37    = 397.949
hW38    = 397.949
hW39    = 397.949

hW40    = 397.949
hW41    = 397.949
hW42    = 397.949
hW43    = 397.949
hW44    = 397.949
hW45    = 397.949
hW46    = 397.949
hW47    = 397.949

hW48    = 397.949
hW49    = 397.949
hW50    = 397.949
hW51    = 397.949
hW52    = 397.949
hW53    = 397.949
hW54    = 397.949
hW55    = 397.949

hW56    = 397.949
hW57    = 397.949
hW58    = 397.949
hW59    = 397.949
hW60    = 397.949
hW61    = 397.949
hW62    = 397.949
hW63    = 397.949

hW64    = m.Var(lb=83.799,ub=418.892)
hW65    = m.Var(lb=83.799,ub=418.892)
hW66    = m.Var(lb=83.799,ub=418.892)

hW67    = m.Var(lb=83.799,ub=418.892)
hW67MED = m.Var(lb=83.799,ub=418.892)
hW67MED1 = m.Var(lb=418.892,ub=2662)
hW67MED2 = m.Var(lb=418.892,ub=2662)
hW67MED3 = m.Var(lb=418.892,ub=2662)
hW67MED4 = m.Var(lb=418.892,ub=2662)

hW68    = 418.892

hW69    = 418.892
hW70    = 418.892
hW71    = 418.892
hW72    = 418.892
hW73    = 418.892
hW74    = 418.892
hW75    = 418.892
hW76    = 418.892


hW79    = 418.892
hW80    = 418.892
hW81    = 418.892

hW82    = m.Var(lb=139.634,ub=418.892)
hW83    = m.Var(lb=139.634,ub=418.892)
hW84    = m.Var(lb=139.634,ub=418.892)


hW85    = m.Var(lb=139.634,ub=418.892)
hW86    = m.Var(lb=139.634,ub=418.892)
hW87    = m.Var(lb=139.634,ub=418.892)

hW88    = m.Var(lb=139.634,ub=418.892)
hW89    = m.Var(lb=139.634,ub=418.892)
hW90    = m.Var(lb=139.634,ub=418.892)

hW91    = m.Var(lb=139.634,ub=418.892)
hW92    = m.Var(lb=139.634,ub=418.892)
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```
hW93    = m.Var(lb=139.634,ub=418.892)

hW94    = m.Var(lb=139.634,ub=418.892)
hW95    = m.Var(lb=139.634,ub=418.892)
hW96    = m.Var(lb=139.634,ub=418.892)

hW97    = m.Var(lb=139.634,ub=418.892)
hW98    = 139.634






CW1A1     = 0.00

CW1A2     = 0.00
CW1A3     = 0.00
CW1A3A   = 0.00

CW1A4     = 0.00
CW1A5     = 0.00
CW1A6     = 0.00
CW1A7     = 0.00
CW1A8     = 0.00

CW1A9     = 0.00
CW1A10    = 0.00
CW1A11    = 0.00
CW1A12    = 0.00
CW1A13    = 0.00

CW1A14    = 0.00
CW1A15    = 0.00
CW1A16    = 0.00
CW1A17    = 0.00
CW1A18    = 0.00

CW1A19    = m.Var(lb=0.00,ub=500.00)
CW1A20    = m.Var(lb=0.00,ub=500.00)
CW1A21    = m.Var(lb=0.00,ub=500.00)

CW1A22    = m.Var(lb=0.00,ub=500.00)
CW1A23    = m.Var(lb=0.00,ub=500.00)
CW1A24    = m.Var(lb=0.00,ub=500.00)

CW1A25    = m.Var(lb=0.00,ub=500.00)
CW1A26    = m.Var(lb=0.00,ub=500.00)
CW1A27    = m.Var(lb=0.00,ub=500.00)

CW1A28    = m.Var(lb=0.00,ub=500.00)
CW1A29    = m.Var(lb=0.00,ub=500.00)
CW1A30    = m.Var(lb=0.00,ub=500.00)

CW1A31    = m.Var(lb=0.00,ub=500.00)
CW1A32    = m.Var(lb=0.00,ub=500.00)
CW1A33    = m.Var(lb=0.00,ub=500.00)

CW1A34    = m.Var(lb=0.00,ub=500.00)
CW1A35    = m.Var(lb=0.00,ub=500.00)
CW1A36    = m.Var(lb=0.00,ub=500.00)

CW1A37    = m.Var(lb=800.00,ub=1000.00)
CW1A38    = m.Var(lb=800.00,ub=1000.00)
CW1A39    = m.Var(lb=800.00,ub=1000.00)

CW1A40    = m.Var(lb=800.00,ub=1000.00)
CW1A41    = m.Var(lb=800.00,ub=1000.00)
CW1A42    = m.Var(lb=800.00,ub=1000.00)
CW1A43    = m.Var(lb=800.00,ub=1000.00)
CW1A44    = m.Var(lb=800.00,ub=1000.00)
CW1A45    = m.Var(lb=800.00,ub=1000.00)
CW1A46    = m.Var(lb=800.00,ub=1000.00)
CW1A47    = m.Var(lb=800.00,ub=1000.00)

CW1A48    = m.Var(lb=800.00,ub=1000.00)
CW1A49    = m.Var(lb=800.00,ub=1000.00)
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```
CW1A50    = m.Var(lb=800.00,ub=1000.00)
CW1A51    = m.Var(lb=800.00,ub=1000.00)
CW1A52    = m.Var(lb=800.00,ub=1000.00)
CW1A53    = m.Var(lb=800.00,ub=1000.00)
CW1A54    = m.Var(lb=800.00,ub=1000.00)
CW1A55    = m.Var(lb=800.00,ub=1000.00)

CW1A56    = m.Var(lb=800.00,ub=1000.00)
CW1A57    = m.Var(lb=800.00,ub=1000.00)
CW1A58    = m.Var(lb=800.00,ub=1000.00)
CW1A59    = m.Var(lb=800.00,ub=1000.00)
CW1A60    = m.Var(lb=800.00,ub=1000.00)
CW1A61    = m.Var(lb=800.00,ub=1000.00)
CW1A62    = m.Var(lb=800.00,ub=1000.00)
CW1A63    = m.Var(lb=800.00,ub=1000.00)

CW1A64    = m.Var(lb=0.00,ub=1000.00)
CW1A65    = m.Var(lb=0.00,ub=1000.00)
CW1A66    = m.Var(lb=0.00,ub=1000.00)

CW1A67    = m.Var(lb=0.00,ub=1000.00)

CF1A1     = m.Var(lb=0.00)



CW1A68    = 0.00

CW1A69    = 0.00
CW1A70    = 0.00
CW1A71    = 0.00
CW1A72    = 0.00
CW1A73    = 0.00
CW1A74    = 0.00
CW1A75    = 0.00
CW1A76    = 0.00


CW1A79    = 0.00
CW1A80    = 0.00
CW1A81    = 0.00

CW1A82    = m.Var(lb=0.00,ub=1000.00)
CW1A83    = m.Var(lb=0.00,ub=1000.00)
CW1A84    = m.Var(lb=0.00,ub=1000.00)


CW1A85    = m.Var(lb=0.00,ub=1000.00)
CW1A86    = m.Var(lb=0.00,ub=1000.00)
CW1A87    = m.Var(lb=0.00,ub=1000.00)

CW1A88    = m.Var(lb=0.00,ub=1000.00)
CW1A89    = m.Var(lb=0.00,ub=1000.00)
CW1A90    = m.Var(lb=0.00,ub=1000.00)

CW1A91    = m.Var(lb=0.00,ub=1000.00)
CW1A92    = m.Var(lb=0.00,ub=1000.00)
CW1A93    = m.Var(lb=0.00,ub=1000.00)

CW1A94    = m.Var(lb=0.00,ub=1000.00)
CW1A95    = m.Var(lb=0.00,ub=1000.00)
CW1A96    = m.Var(lb=0.00,ub=1000.00)

CW1A97    = m.Var(lb=0.00,ub=1000.00)
CW1A98    = m.Var(lb=0.00,ub=1000.00)






CW2A1     = 0.00

CW2A2     = 0.00
CW2A3     = 0.00
CW2A3A   = 0.00
```

```
CW2A4      = 0.00
CW2A5      = 0.00
CW2A6      = 0.00
CW2A7      = 0.00
CW2A8      = 0.00

CW2A9      = 0.00
CW2A10     = 0.00
CW2A11     = 0.00
CW2A12     = 0.00
CW2A13     = 0.00

CW2A14     = 0.00
CW2A15     = 0.00
CW2A16     = 0.00
CW2A17     = 0.00
CW2A18     = 0.00

CW2A19     = m.Var(lb=0.00,ub=2000.00)
CW2A20     = m.Var(lb=0.00,ub=2000.00)
CW2A21     = m.Var(lb=0.00,ub=2000.00)

CW2A22     = m.Var(lb=0.00,ub=2000.00)
CW2A23     = m.Var(lb=0.00,ub=2000.00)
CW2A24     = m.Var(lb=0.00,ub=2000.00)

CW2A25     = m.Var(lb=0.00,ub=2000.00)
CW2A26     = m.Var(lb=0.00,ub=2000.00)
CW2A27     = m.Var(lb=0.00,ub=2000.00)

CW2A28     = m.Var(lb=0.00,ub=2000.00)
CW2A29     = m.Var(lb=0.00,ub=2000.00)
CW2A30     = m.Var(lb=0.00,ub=2000.00)

CW2A31     = m.Var(lb=0.00,ub=2000.00)
CW2A32     = m.Var(lb=0.00,ub=2000.00)
CW2A33     = m.Var(lb=0.00,ub=2000.00)

CW2A34     = m.Var(lb=0.00,ub=300.00)
CW2A35     = m.Var(lb=0.00,ub=300.00)
CW2A36     = m.Var(lb=0.00,ub=300.00)

CW2A37     = m.Var(lb=800.00,ub=1000.00)
CW2A38     = m.Var(lb=800.00,ub=1000.00)
CW2A39     = m.Var(lb=800.00,ub=1000.00)

CW2A40     = m.Var(lb=800.00,ub=1000.00)
CW2A41     = m.Var(lb=800.00,ub=1000.00)
CW2A42     = m.Var(lb=800.00,ub=1000.00)
CW2A43     = m.Var(lb=800.00,ub=1000.00)
CW2A44     = m.Var(lb=800.00,ub=1000.00)
CW2A45     = m.Var(lb=800.00,ub=1000.00)
CW2A46     = m.Var(lb=800.00,ub=1000.00)
CW2A47     = m.Var(lb=800.00,ub=1000.00)

CW2A48     = m.Var(lb=800.00,ub=1000.00)
CW2A49     = m.Var(lb=800.00,ub=1000.00)
CW2A50     = m.Var(lb=800.00,ub=1000.00)
CW2A51     = m.Var(lb=800.00,ub=1000.00)
CW2A52     = m.Var(lb=800.00,ub=1000.00)
CW2A53     = m.Var(lb=800.00,ub=1000.00)
CW2A54     = m.Var(lb=800.00,ub=1000.00)
CW2A55     = m.Var(lb=800.00,ub=1000.00)

CW2A56     = m.Var(lb=800.00,ub=1000.00)
CW2A57     = m.Var(lb=800.00,ub=1000.00)
CW2A58     = m.Var(lb=800.00,ub=1000.00)
CW2A59     = m.Var(lb=800.00,ub=1000.00)
CW2A60     = m.Var(lb=800.00,ub=1000.00)
CW2A61     = m.Var(lb=800.00,ub=1000.00)
CW2A62     = m.Var(lb=800.00,ub=1000.00)
CW2A63     = m.Var(lb=800.00,ub=1000.00)

CW2A64     = m.Var(lb=0.00,ub=2000.00)
CW2A65     = m.Var(lb=0.00,ub=2000.00)
CW2A66     = m.Var(lb=0.00,ub=2000.00)
```

```
CW2A67    = m.Var(lb=0.00,ub=2000.00)

CF2A1     = m.Var(lb=0.00,ub=10000000.00)


CW2A68    = 0.00

CW2A69    = 0.00
CW2A70    = 0.00
CW2A71    = 0.00
CW2A72    = 0.00
CW2A73    = 0.00
CW2A74    = 0.00
CW2A75    = 0.00
CW2A76    = 0.00


CW2A79    = 0.00
CW2A80    = 0.00
CW2A81    = 0.00

CW2A82    = m.Var(lb=0.00,ub=2000.00)
CW2A83    = m.Var(lb=0.00,ub=2000.00)
CW2A84    = m.Var(lb=0.00,ub=2000.00)


CW2A85    = m.Var(lb=0.00,ub=2000.00)
CW2A86    = m.Var(lb=0.00,ub=2000.00)
CW2A87    = m.Var(lb=0.00,ub=2000.00)

CW2A88    = m.Var(lb=0.00,ub=2000.00)
CW2A89    = m.Var(lb=0.00,ub=2000.00)
CW2A90    = m.Var(lb=0.00,ub=2000.00)

CW2A91    = m.Var(lb=0.00,ub=2000.00)
CW2A92    = m.Var(lb=0.00,ub=2000.00)
CW2A93    = m.Var(lb=0.00,ub=2000.00)

CW2A94    = m.Var(lb=0.00,ub=2000.00)
CW2A95    = m.Var(lb=0.00,ub=2000.00)
CW2A96    = m.Var(lb=0.00,ub=2000.00)

CW2A97    = m.Var(lb=0.00,ub=2000.00)
CW2A98    = m.Var(lb=0.00,ub=2000.00)




CW3A1     = 0.00

CW3A2     = 0.00
CW3A3     = 0.00
CW3A3A   = 0.00

CW3A4     = 0.00
CW3A5     = 0.00
CW3A6     = 0.00
CW3A7     = 0.00
CW3A8     = 0.00

CW3A9     = 0.00
CW3A10    = 0.00
CW3A11    = 0.00
CW3A12    = 0.00
CW3A13    = 0.00

CW3A14    = 0.00
CW3A15    = 0.00
CW3A16    = 0.00
CW3A17    = 0.00
CW3A18    = 0.00

CW3A19    = m.Var(lb=0.00,ub=200.00)
CW3A20    = m.Var(lb=0.00,ub=200.00)
CW3A21    = m.Var(lb=0.00,ub=200.00)
```

```
CW3A22    = m.Var(lb=0.00,ub=200.00)
CW3A23    = m.Var(lb=0.00,ub=200.00)
CW3A24    = m.Var(lb=0.00,ub=200.00)

CW3A25    = m.Var(lb=0.00,ub=200.00)
CW3A26    = m.Var(lb=0.00,ub=200.00)
CW3A27    = m.Var(lb=0.00,ub=200.00)

CW3A28    = m.Var(lb=0.00,ub=200.00)
CW3A29    = m.Var(lb=0.00,ub=200.00)
CW3A30    = m.Var(lb=0.00,ub=200.00)

CW3A31    = m.Var(lb=0.00,ub=200.00)
CW3A32    = m.Var(lb=0.00,ub=200.00)
CW3A33    = m.Var(lb=0.00,ub=200.00)

CW3A34    = m.Var(lb=0.00,ub=200.00)
CW3A35    = m.Var(lb=0.00,ub=200.00)
CW3A36    = m.Var(lb=0.00,ub=200.00)

CW3A37    = m.Var(lb=800.00,ub=1000.00)
CW3A38    = m.Var(lb=800.00,ub=1000.00)
CW3A39    = m.Var(lb=800.00,ub=1000.00)

CW3A40    = m.Var(lb=800.00,ub=1000.00)
CW3A41    = m.Var(lb=800.00,ub=1000.00)
CW3A42    = m.Var(lb=800.00,ub=1000.00)
CW3A43    = m.Var(lb=800.00,ub=1000.00)
CW3A44    = m.Var(lb=800.00,ub=1000.00)
CW3A45    = m.Var(lb=800.00,ub=1000.00)
CW3A46    = m.Var(lb=800.00,ub=1000.00)
CW3A47    = m.Var(lb=800.00,ub=1000.00)

CW3A48    = m.Var(lb=800.00,ub=1000.00)
CW3A49    = m.Var(lb=800.00,ub=1000.00)
CW3A50    = m.Var(lb=800.00,ub=1000.00)
CW3A51    = m.Var(lb=800.00,ub=1000.00)
CW3A52    = m.Var(lb=800.00,ub=1000.00)
CW3A53    = m.Var(lb=800.00,ub=1000.00)
CW3A54    = m.Var(lb=800.00,ub=1000.00)
CW3A55    = m.Var(lb=800.00,ub=1000.00)

CW3A56    = m.Var(lb=800.00,ub=1000.00)
CW3A57    = m.Var(lb=800.00,ub=1000.00)
CW3A58    = m.Var(lb=800.00,ub=1000.00)
CW3A59    = m.Var(lb=800.00,ub=1000.00)
CW3A60    = m.Var(lb=800.00,ub=1000.00)
CW3A61    = m.Var(lb=800.00,ub=1000.00)
CW3A62    = m.Var(lb=800.00,ub=1000.00)
CW3A63    = m.Var(lb=800.00,ub=1000.00)

CW3A64    = m.Var(lb=0.00,ub=1000.00)
CW3A65    = m.Var(lb=0.00,ub=1000.00)
CW3A66    = m.Var(lb=0.00,ub=1000.00)

CW3A67    = m.Var(lb=0.00,ub=1000.00)

CF3A1     = m.Var(lb=0.00,ub=10000000.00)


CW3A68    = 0.00

CW3A69    = 0.00
CW3A70    = 0.00
CW3A71    = 0.00
CW3A72    = 0.00
CW3A73    = 0.00
CW3A74    = 0.00
CW3A75    = 0.00
CW3A76    = 0.00


CW3A79    = 0.00
CW3A80    = 0.00
CW3A81    = 0.00

CW3A82    = m.Var(lb=0.00,ub=1000.00)
```

```
CW3A83    = m.Var(lb=0.00,ub=1000.00)
CW3A84    = m.Var(lb=0.00,ub=1000.00)


CW3A85    = m.Var(lb=0.00,ub=1000.00)
CW3A86    = m.Var(lb=0.00,ub=1000.00)
CW3A87    = m.Var(lb=0.00,ub=1000.00)

CW3A88    = m.Var(lb=0.00,ub=1000.00)
CW3A89    = m.Var(lb=0.00,ub=1000.00)
CW3A90    = m.Var(lb=0.00,ub=1000.00)

CW3A91    = m.Var(lb=0.00,ub=1000.00)
CW3A92    = m.Var(lb=0.00,ub=1000.00)
CW3A93    = m.Var(lb=0.00,ub=1000.00)

CW3A94    = m.Var(lb=0.00,ub=1000.00)
CW3A95    = m.Var(lb=0.00,ub=1000.00)
CW3A96    = m.Var(lb=0.00,ub=1000.00)

CW3A97    = m.Var(lb=0.00,ub=1000.00)
CW3A98    = m.Var(lb=0.00,ub=1000.00)



q1        = m.Var(lb=0.00,ub=100000000)
q2        = m.Var(lb=0.00,ub=100000000)
q3        = m.Var(lb=0.00,ub=100000000)

qC1        = m.Var(lb=0.00,ub=100000000)
qC2        = m.Var(lb=0.00,ub=100000000)
qC3        = m.Var(lb=0.00,ub=100000000)




qTotal    = m.Var(lb=0.00,ub=10000000.00)


qCTotal   = m.Var(lb=0.00,ub=10000000.00)


##################################################################################


MAir10   = 21622.1
MAir20   = 16528.4


MAir1     = m.Var(lb=0.00,ub=21622.1)
MAir2     = 0.00


MAir1Out     = m.Var(lb=0.00,ub=21622.1)
MAir2Out     = m.Var(lb=0.00,ub=16528.4)


MAir   = m.Var(lb=0.00,ub=38150.5)

MAirMED   = m.Var(lb=0.00,ub=38150.5)
MAirOut   = m.Var(lb=0.00,ub=38150.5)

MAirOut1   = m.Var(lb=0.00,ub=38150.5)
MAirOut2   = m.Var(lb=0.00,ub=38150.5)
MAirOut3   = m.Var(lb=0.00,ub=38150.5)

MAirOutOut   = m.Var(lb=0.00,ub=38150.5)



TAir1     = 111.4664007
TAir2     = 196.4541386

TAir      = m.Var(lb=111.4664007,ub=196.4541386)
```

```
TAirMEDInt= m.Var(lb=35.00,ub=196.4541386)


TAirMEDOut= m.Var(lb=35.00,ub=196.4541386)



hAir1      = 384.414448749
hAir2      = 475.351328302

hAir       = m.Var(lb=384.414448749,ub=475.351328302)






hAirMEDInt = m.Var(lb=302.5954,ub=475.351328302)

hAirMEDOut = m.Var(lb=302.5954,ub=475.351328302)


TAirOut1   = m.Var(lb=35.00,ub=196.4541386)
TAirOut2   = m.Var(lb=35.00,ub=196.4541386)
TAirOut3   = m.Var(lb=35.00,ub=196.4541386)
TAirOutOut = m.Var(lb=35.00,ub=196.4541386)


hAirOut1   = m.Var(lb=302.5954,ub=475.351328302)
hAirOut2   = m.Var(lb=302.5954,ub=475.351328302)
hAirOut3   = m.Var(lb=302.5954,ub=475.351328302)
hAirOutOut = m.Var(lb=302.5954,ub=475.351328302)


qMED = m.Var(lb=0.00,ub=1000000.00)

qLoss = m.Var(lb=0.00,ub=1000000.00)

AHMED = m.Var(lb=0.00,ub=1000000.00)





qH1 = m.Var(lb=0.00,ub=1000000.00)
qH2 = m.Var(lb=0.00,ub=1000000.00)
qH3 = m.Var(lb=0.00,ub=1000000.00)

AH1 = m.Var(lb=0.00,ub=100000.00)
AH2 = m.Var(lb=0.00,ub=100000.00)
AH3 = m.Var(lb=0.00,ub=100000.00)


#################################################################################


# Constraints

## Water System



m.Equation(MW1 == MW2 + MW3 + MW3A)



m.Equation(MW2 == MW4 + MW5 + MW6 + MW7 + MW8)

m.Equation(MW3 == MW9 + MW10 + MW11 + MW12 + MW13)

m.Equation(MW3A == MW14 + MW15 + MW16 + MW17 + MW18)



m.Equation(MW4 +  MW41 + MW49 + MW57 + MW70 == MW19)
m.Equation(MW4 * hW4 +  MW41 * hW41 + MW49 * hW49 + MW57 * hW57 + MW70 * hW70 == MW19 *
```

```
hW19)
m.Equation(MW4 * CW1A4 +  MW41 * CW1A41 + MW49 * CW1A49 + MW57 * CW1A57 + MW70 * CW1A70
== MW19 * CW1A19)
m.Equation(MW4 * CW2A4 +  MW41 * CW2A41 + MW49 * CW2A49 + MW57 * CW2A57 + MW70 * CW2A70
== MW19 * CW2A19)
m.Equation(MW4 * CW3A4 +  MW41 * CW3A41 + MW49 * CW3A49 + MW57 * CW3A57 + MW70 * CW3A70
== MW19 * CW3A19)

m.Equation(MW9 + MW42 + MW50 + MW58 + MW71 == MW20)
m.Equation(MW9 * hW9 + MW42 * hW42 + MW50 * hW50 + MW58 * hW58 + MW71 * hW71 == MW20 *
hW20)
m.Equation(MW9 * CW1A9 + MW42 * CW1A42 + MW50 * CW1A50 + MW58 * CW1A58 + MW71 * CW1A71
== MW20 * CW1A20)
m.Equation(MW9 * CW2A9 + MW42 * CW2A42 + MW50 * CW2A50 + MW58 * CW2A58 + MW71 * CW2A71
== MW20 * CW2A20)
m.Equation(MW9 * CW3A9 + MW42 * CW3A42 + MW50 * CW3A50 + MW58 * CW3A58 + MW71 * CW3A71
== MW20 * CW3A20)

m.Equation(MW14 + MW43 + MW51 + MW59 + MW72 == MW21)
m.Equation(MW14 * hW14 + MW43 * hW43 + MW51 * hW51 + MW59 * hW59 + MW72 * hW72 == MW21
* hW21)
m.Equation(MW14 * CW1A14 + MW43 * CW1A43 + MW51 * CW1A51 + MW59 * CW1A59 + MW72 *
CW1A72 == MW21 * CW1A21)
m.Equation(MW14 * CW2A14 + MW43 * CW2A43 + MW51 * CW2A51 + MW59 * CW2A59 + MW72 *
CW2A72 == MW21 * CW2A21)
m.Equation(MW14 * CW3A14 + MW43 * CW3A43 + MW51 * CW3A51 + MW59 * CW3A59 + MW72 *
CW3A72 == MW21 * CW3A21)




m.Equation(MW19 * (hW19A - hW19) == qH1)
m.Equation(qH1 * (1000 / 3600) == 400 * AH1 * (((TAir - TW19A) * (TAirOut1 - TW19) *
((TAir - TW19A) + (TAirOut1 - TW19)) * 0.5) ** (1/3)))

m.Equation(MW20 * (hW20A - hW20) == qH2)
m.Equation(qH2 * (1000 / 3600) == 400 * AH2 * (((TAir - TW20A) * (TAirOut2 - TW20) *
((TAir - TW20A) + (TAirOut2 - TW20)) * 0.5) ** (1/3)))

m.Equation(MW21 * (hW21A - hW21) == qH3)
m.Equation(qH3 * (1000 / 3600) == 400 * AH3 * (((TAir - TW21A) * (TAirOut3 - TW21) *
((TAir - TW21A) + (TAirOut3 - TW21)) * 0.5) ** (1/3)))



m.Equation(MW19 == MW22)
m.Equation(MW19 * hW19A + q1 * 0.779 == MW22 * hW22)
m.Equation(CW1A19 == CW1A22)
m.Equation(CW2A19 == CW2A22)
m.Equation(CW3A19 == CW3A22)

m.Equation(MW20 == MW23)
m.Equation(MW20 * hW20A + q2 * 0.847 == MW23 * hW23)
m.Equation(CW1A20 == CW1A23)
m.Equation(CW2A20 == CW2A23)
m.Equation(CW3A20 == CW3A23)

m.Equation(MW21 == MW24)
m.Equation(MW21 * hW21A + q3 * 0.594 == MW24 * hW24)
m.Equation(CW1A21 == CW1A24)
m.Equation(CW2A21 == CW2A24)
m.Equation(CW3A21 == CW3A24)




m.Equation(MW22 == MW25 + MW26 + MW27)
m.Equation(hW22 == hW25)
m.Equation(hW22 == hW26)
m.Equation(hW22 == hW27)


m.Equation(CW1A22 == CW1A25)
m.Equation(CW2A22 == CW2A25)
```

```
m.Equation(CW3A22 == CW3A25)
m.Equation(CW1A22 == CW1A26)
m.Equation(CW2A22 == CW2A26)
m.Equation(CW3A22 == CW3A26)
m.Equation(CW1A22 == CW1A27)
m.Equation(CW2A22 == CW2A27)
m.Equation(CW3A22 == CW3A27)



m.Equation(MW23 == MW28 + MW29 + MW30)
m.Equation(hW23 == hW28)
m.Equation(hW23 == hW29)
m.Equation(hW23 == hW30)



m.Equation(CW1A23 == CW1A28)
m.Equation(CW2A23 == CW2A28)
m.Equation(CW3A23 == CW3A28)
m.Equation(CW1A23 == CW1A29)
m.Equation(CW2A23 == CW2A29)
m.Equation(CW3A23 == CW3A29)
m.Equation(CW1A23 == CW1A30)
m.Equation(CW2A23 == CW2A30)
m.Equation(CW3A23 == CW3A30)




m.Equation(MW24 == MW31 + MW32 + MW33)
m.Equation(hW24 == hW31)
m.Equation(hW24 == hW32)
m.Equation(hW24 == hW33)



m.Equation(CW1A24 == CW1A31)
m.Equation(CW2A24 == CW2A31)
m.Equation(CW3A24 == CW3A31)
m.Equation(CW1A24 == CW1A32)
m.Equation(CW2A24 == CW2A32)
m.Equation(CW3A24 == CW3A32)
m.Equation(CW1A24 == CW1A33)
m.Equation(CW2A24 == CW2A33)
m.Equation(CW3A24 == CW3A33)




m.Equation(MW25 + MW6 + MW73 + MW89 == MW34)
m.Equation(MW25 * hW25 + MW6 * hW6 + MW73 * hW73 + MW89 * hW89 == MW34 * hW34)
m.Equation(MW25 * CW1A25 + MW6 * CW1A6 + MW73 * CW1A73 + MW89 * CW1A89 == MW34 *
CW1A34)
m.Equation(MW25 * CW2A25 + MW6 * CW2A6 + MW73 * CW2A73 + MW89 * CW2A89 == MW34 *
CW2A34)
m.Equation(MW25 * CW3A25 + MW6 * CW3A6 + MW73 * CW3A73 + MW89 * CW3A89 == MW34 *
CW3A34)

m.Equation(MW28 + MW11 + MW74 + MW92 == MW35)
m.Equation(MW28 * hW28 + MW11 * hW11 + MW74 * hW74 + MW92 * hW92 == MW35 * hW35)
m.Equation(MW28 * CW1A28 + MW11 * CW1A11 + MW74 * CW1A74 + MW92 * CW1A92 == MW35 *
CW1A35)
m.Equation(MW28 * CW2A28 + MW11 * CW2A11 + MW74 * CW2A74 + MW92 * CW2A92 == MW35 *
CW2A35)
m.Equation(MW28 * CW3A28 + MW11 * CW3A11 + MW74 * CW3A74 + MW92 * CW3A92 == MW35 *
CW3A35)

m.Equation(MW31 + MW16 + MW75 + MW95 == MW36)
m.Equation(MW31 * hW31 + MW16 * hW16 + MW75 * hW75 + MW95 * hW95 == MW36 * hW36)
m.Equation(MW31 * CW1A31 + MW16 * CW1A16 + MW75 * CW1A75 + MW95 * CW1A95 == MW36 *
CW1A36)
m.Equation(MW31 * CW2A31 + MW16 * CW2A16 + MW75 * CW2A75 + MW95 * CW2A95 == MW36 *
CW2A36)
m.Equation(MW31 * CW3A31 + MW16 * CW3A16 + MW75 * CW3A75 + MW95 * CW3A95 == MW36 *
CW3A36)
```

```
m.Equation(MW34 == MW37)
m.Equation(MW34 * (CW1A34 * (10 ** -6)) + 0.249117072 == MW37 * (CW1A37 * (10 ** -6)))
m.Equation(MW34 * (CW2A34 * (10 ** -6)) + 0.249117072 == MW37 * (CW2A37 * (10 ** -6)))
m.Equation(MW34 * (CW3A34 * (10 ** -6)) + 0.249117072 == MW37 * (CW3A37 * (10 ** -6)))

m.Equation(MW35 == MW38)
m.Equation(MW35 * (CW1A35 * (10 ** -6)) + 0.388756392 == MW38 * (CW1A38 * (10 ** -6)))
m.Equation(MW35 * (CW2A35 * (10 ** -6)) + 0.388756392 == MW38 * (CW2A38 * (10 ** -6)))
m.Equation(MW35 * (CW3A35 * (10 ** -6)) + 0.388756392 == MW38 * (CW3A38 * (10 ** -6)))

m.Equation(MW36 == MW39)
m.Equation(MW36 * (CW1A36 * (10 ** -6)) + 0.049880471 == MW39 * (CW1A39 * (10 ** -6)))
m.Equation(MW36 * (CW2A36 * (10 ** -6)) + 0.049880471 == MW39 * (CW2A39 * (10 ** -6)))
m.Equation(MW36 * (CW3A36 * (10 ** -6)) + 0.049880471 == MW39 * (CW3A39 * (10 ** -6)))



m.Equation(MW37 == MW40 + MW41 + MW42 + MW43 + MW44 + MW45 + MW46 + MW47)
m.Equation(CW1A37 == CW1A40)
m.Equation(CW1A37 == CW1A41)
m.Equation(CW1A37 == CW1A42)
m.Equation(CW1A37 == CW1A43)
m.Equation(CW1A37 == CW1A44)
m.Equation(CW1A37 == CW1A45)
m.Equation(CW1A37 == CW1A46)
m.Equation(CW1A37 == CW1A47)

m.Equation(MW38 == MW48 + MW49 + MW50 + MW51 + MW52 + MW53 + MW54 + MW55)
m.Equation(CW1A38 == CW1A48)
m.Equation(CW1A38 == CW1A49)
m.Equation(CW1A38 == CW1A50)
m.Equation(CW1A38 == CW1A51)
m.Equation(CW1A38 == CW1A52)
m.Equation(CW1A38 == CW1A53)
m.Equation(CW1A38 == CW1A54)
m.Equation(CW1A38 == CW1A55)

m.Equation(MW39 == MW56 + MW57 + MW58 + MW59 + MW60 + MW61 + MW62 + MW63)
m.Equation(CW1A39 == CW1A56)
m.Equation(CW1A39 == CW1A57)
m.Equation(CW1A39 == CW1A58)
m.Equation(CW1A39 == CW1A59)
m.Equation(CW1A39 == CW1A60)
m.Equation(CW1A39 == CW1A61)
m.Equation(CW1A39 == CW1A62)
m.Equation(CW1A39 == CW1A63)



m.Equation(MW40 + MW26 + MW90 + MW5 == MW64)
m.Equation(MW40 * hW40 + MW26 * hW26 + MW90 * hW90 + MW5 * hW5 == MW64 * hW64)
m.Equation(MW40 * CW1A40 + MW26 * CW1A26 + MW90 * CW1A90 + MW5 * CW1A5 == MW64 *
CW1A64)
m.Equation(MW40 * CW2A40 + MW26 * CW2A26 + MW90 * CW2A90 + MW5 * CW2A5 == MW64 *
CW2A64)
m.Equation(MW40 * CW3A40 + MW26 * CW3A26 + MW90 * CW3A90 + MW5 * CW3A5 == MW64 *
CW3A64)

m.Equation(MW48 + MW29 + MW93 + MW10 == MW65)
m.Equation(MW48 * hW48 + MW29 * hW29 + MW93 * hW93 + MW10 * hW10 == MW65 * hW65)
m.Equation(MW48 * CW1A48 + MW29 * CW1A29 + MW93 * CW1A93 + MW10 * CW1A10 == MW65 *
CW1A65)
m.Equation(MW48 * CW2A48 + MW29 * CW2A29 + MW93 * CW2A93 + MW10 * CW2A10 == MW65 *
CW2A65)
m.Equation(MW48 * CW3A48 + MW29 * CW3A29 + MW93 * CW3A93 + MW10 * CW3A10 == MW65 *
CW3A65)

m.Equation(MW56 + MW32 + MW96 + MW15 == MW66)
m.Equation(MW56 * hW56 + MW32 * hW32 + MW96 * hW96 + MW15 * hW15 == MW66 * hW66)
```

```
m.Equation(MW56 * CW1A56 + MW32 * CW1A32 + MW96 * CW1A96 + MW15 * CW1A15 == MW66 *
CW1A66)
m.Equation(MW56 * CW2A56 + MW32 * CW2A32 + MW96 * CW2A96 + MW15 * CW2A15 == MW66 *
CW2A66)
m.Equation(MW56 * CW3A56 + MW32 * CW3A32 + MW96 * CW3A96 + MW15 * CW3A15 == MW66 *
CW3A66)




m.Equation(MW64 + MW65 + MW66 == MW67)
m.Equation(MW64 * hW64 + MW65 * hW65 + MW66 * hW66 == MW67 * hW67)
m.Equation(MW64 * CW1A64 + MW65 * CW1A65 + MW66 * CW1A66 == MW67 * CW1A67)
m.Equation(MW64 * CW2A64 + MW65 * CW2A65 + MW66 * CW2A66 == MW67 * CW2A67)
m.Equation(MW64 * CW3A64 + MW65 * CW3A65 + MW66 * CW3A66 == MW67 * CW3A67)






m.Equation(MW67 == MW67MED)
m.Equation(MW67 * (hW67MED - hW67) == MW67MEDV4 * (hW67MED4 - 418.892) + qLoss)




m.Equation(MW67MED * (1/4) == MW67MEDV1 + MWSludge)
m.Equation(qMED == MW67MEDV1 * (hW67MED1 - 418.892) + MW67MED * (1/4) * (418.892 -
hW67MED))
m.Equation(MW67MED * (1/4) * (hW67MED1 - 418.892) == MW67MEDV1 * (2662 - 418.892))


m.Equation(MW67MEDV1 * (hW67MED1 - 418.892) * (1000 / 3600) == 400 * AHMED * (((TAir -
100.00) * (TAirMEDInt - 100.00) * ((TAir - 100.00) + (TAirMEDInt - 100.00)) * 0.5) **
(1 / 3)))





m.Equation(MW67MED * (1/4) == MW67MEDV2 + MWSludge2)
m.Equation(MW67MEDV1 * (hW67MED1 - 418.892) == MW67MEDV2 * (hW67MED2 - 418.892) +
MW67MED * (1/4) * (418.892 - hW67MED))
m.Equation(MW67MED * (1/4) * (hW67MED2 - 418.892) == MW67MEDV2 * (2662 - 418.892))


m.Equation(MW67MED * (1/4) == MW67MEDV3 + MWSludge3)
m.Equation(MW67MEDV2 * (hW67MED2 - 418.892) == MW67MEDV3 * (hW67MED3 - 418.892) +
MW67MED * (1/4) * (418.892 - hW67MED))
m.Equation(MW67MED * (1/4) * (hW67MED3 - 418.892) == MW67MEDV3 * (2662 - 418.892))

m.Equation(MW67MED * (1/4) == MW67MEDV4 + MWSludge4)
m.Equation(MW67MEDV3 * (hW67MED3 - 418.892) == MW67MEDV4 * (hW67MED4 - 418.892) +
MW67MED * (1/4) * (418.892 - hW67MED))
m.Equation(MW67MED * (1/4) * (hW67MED4 - 418.892) == MW67MEDV4 * (2662 - 418.892))





m.Equation(MW67MEDV1 + MW67MEDV2 + MW67MEDV3 + MW67MEDV4 == MW68)


m.Equation(MW67 == MW68 + MF1)
m.Equation(MW67 * CW1A67 == MW68 * CW1A68 + MF1 * CF1A1)
m.Equation(MW67 * CW2A67 == MW68 * CW2A68 + MF1 * CF2A1)
m.Equation(MW67 * CW3A67 == MW68 * CW3A68 + MF1 * CF3A1)



m.Equation(MW68 == MW69 + MW70 + MW71 + MW72 + MW73 + MW74 + MW75 + MW76)



m.Equation(MW69 == MW79 + MW80 + MW81)
```

```
m.Equation(MW79 + MW44 + MW52 + MW60 + MW7 == MW82)
m.Equation(MW79 * hW79 + MW44 * hW44 + MW52 * hW52 + MW60 * hW60 + MW7 * hW7 == MW82 *
hW82)
m.Equation(MW79 * CW1A79 + MW44 * CW1A44 + MW52 * CW1A52 + MW60 * CW1A60 + MW7 * CW1A7
== MW82 * CW1A82)
m.Equation(MW79 * CW2A79 + MW44 * CW2A44 + MW52 * CW2A52 + MW60 * CW2A60 + MW7 * CW2A7
== MW82 * CW2A82)
m.Equation(MW79 * CW3A79 + MW44 * CW3A44 + MW52 * CW3A52 + MW60 * CW3A60 + MW7 * CW3A7
== MW82 * CW3A82)

m.Equation(MW80 + MW45 + MW53 + MW61 + MW12 == MW83)
m.Equation(MW80 * hW80 + MW45 * hW45 + MW53 * hW53 + MW61 * hW61 + MW12 * hW12 == MW83
* hW83)
m.Equation(MW80 * CW1A80 + MW45 * CW1A45 + MW53 * CW1A53 + MW61 * CW1A61 + MW12 *
CW1A12 == MW83 * CW1A83)
m.Equation(MW80 * CW2A80 + MW45 * CW2A45 + MW53 * CW2A53 + MW61 * CW2A61 + MW12 *
CW2A12 == MW83 * CW2A83)
m.Equation(MW80 * CW3A80 + MW45 * CW3A45 + MW53 * CW3A53 + MW61 * CW3A61 + MW12 *
CW3A12 == MW83 * CW3A83)

m.Equation(MW81 + MW46 + MW54 + MW62 + MW16 == MW84)
m.Equation(MW81 * hW81 + MW46 * hW46 + MW54 * hW54 + MW62 * hW62 + MW16 * hW16 == MW84
* hW84)
m.Equation(MW81 * CW1A81 + MW46 * CW1A46 + MW54 * CW1A54 + MW62 * CW1A62 + MW16 *
CW1A16 == MW84 * CW1A84)
m.Equation(MW81 * CW2A81 + MW46 * CW2A46 + MW54 * CW2A54 + MW62 * CW2A62 + MW16 *
CW2A16 == MW84 * CW2A84)
m.Equation(MW81 * CW3A81 + MW46 * CW3A46 + MW54 * CW3A54 + MW62 * CW3A62 + MW16 *
CW3A16 == MW84 * CW3A84)



m.Equation(MW82 == MW85)
m.Equation(MW82 * hW82 == MW85 * hW85 + qC1)
m.Equation(CW1A82 == CW1A85)
m.Equation(CW2A82 == CW2A85)
m.Equation(CW3A82 == CW3A85)

m.Equation(MW83 == MW86)
m.Equation(MW83 * hW83 == MW86 * hW86 + qC2)
m.Equation(CW1A83 == CW1A86)
m.Equation(CW2A83 == CW2A86)
m.Equation(CW3A83 == CW3A86)

m.Equation(MW84 == MW87)
m.Equation(MW84 * hW84 == MW87 * hW87 + qC3)
m.Equation(CW1A84 == CW1A87)
m.Equation(CW2A84 == CW2A87)
m.Equation(CW3A84 == CW3A87)



m.Equation(MW85 == MW88 + MW89 + MW90)

m.Equation(hW85 == hW88)
m.Equation(hW85 == hW89)
m.Equation(hW85 == hW90)


m.Equation(CW1A85 == CW1A88)
m.Equation(CW2A85 == CW2A88)
m.Equation(CW3A85 == CW3A88)
m.Equation(CW1A85 == CW1A89)
m.Equation(CW2A85 == CW2A89)
m.Equation(CW3A85 == CW3A89)
m.Equation(CW1A85 == CW1A90)
m.Equation(CW2A85 == CW2A90)
m.Equation(CW3A85 == CW3A90)
```

```
m.Equation(MW86 == MW91 + MW92 + MW93)

m.Equation(hW86 == hW91)
m.Equation(hW86 == hW92)
m.Equation(hW86 == hW93)

m.Equation(CW1A86 == CW1A91)
m.Equation(CW2A86 == CW2A91)
m.Equation(CW3A86 == CW3A91)
m.Equation(CW1A86 == CW1A92)
m.Equation(CW2A86 == CW2A92)
m.Equation(CW3A86 == CW3A92)
m.Equation(CW1A86 == CW1A93)
m.Equation(CW2A86 == CW2A93)
m.Equation(CW3A86 == CW3A93)



m.Equation(MW87 == MW94 + MW95 + MW96)

m.Equation(hW87 == hW94)
m.Equation(hW87 == hW95)
m.Equation(hW87 == hW96)


m.Equation(CW1A87 == CW1A94)
m.Equation(CW2A87 == CW2A94)
m.Equation(CW3A87 == CW3A94)
m.Equation(CW1A87 == CW1A95)
m.Equation(CW2A87 == CW2A95)
m.Equation(CW3A87 == CW3A95)
m.Equation(CW1A87 == CW1A96)
m.Equation(CW2A87 == CW2A96)
m.Equation(CW3A87 == CW3A96)



m.Equation(MW88 + MW91 + MW94 == MW97)
m.Equation(MW88 * hW88 + MW91 * hW91 + MW94 * hW94 == MW97 * hW97)
m.Equation(MW88 * CW1A88 + MW91 * CW1A91 + MW94 * CW1A94 == MW97 * CW1A97)
m.Equation(MW88 * CW2A88 + MW91 * CW2A91 + MW94 * CW2A94 == MW97 * CW2A97)
m.Equation(MW88 * CW3A88 + MW91 * CW3A91 + MW94 * CW3A94 == MW97 * CW3A97)



m.Equation(MW97 + MW8 + MW13 + MW18 + MW27 + MW30 + MW33 + MW47 + MW55 + MW63 + MW76 ==
MW98)
m.Equation(MW97 * hW97 + MW8 * hW8 + MW13 * hW13 + MW18 * hW18 + MW27 * hW27 + MW30 *
hW30 + MW33 * hW33 + MW47 * hW47 + MW55 * hW55 + MW63 * hW63 + MW76 * hW76 == MW98 *
hW98)
m.Equation(MW97 * CW1A97 + MW8 * CW1A8 + MW13 * CW1A13 + MW18 * CW1A18 + MW27 * CW1A27
+ MW30 * CW1A30 + MW33 * CW1A33 + MW47 * CW1A47 + MW55 * CW1A55 + MW63 * CW1A63 + MW76
* CW1A76 == MW98 * CW1A98)
m.Equation(MW97 * CW2A97 + MW8 * CW2A8 + MW13 * CW2A13 + MW18 * CW2A18 + MW27 * CW2A27
+ MW30 * CW2A30 + MW33 * CW2A33 + MW47 * CW2A47 + MW55 * CW2A55 + MW63 * CW2A63 + MW76
* CW2A76 == MW98 * CW2A98)
m.Equation(MW97 * CW3A97 + MW8 * CW3A8 + MW13 * CW3A13 + MW18 * CW3A18 + MW27 * CW3A27
+ MW30 * CW3A30 + MW33 * CW3A33 + MW47 * CW3A47 + MW55 * CW3A55 + MW63 * CW3A63 + MW76
* CW3A76 == MW98 * CW3A98)



m.Equation(MW1 == MW98 + MF1)
m.Equation(0.747351216 + 1.166269176 + 0.149641412 == MW98 * ((CW1A98 + CW2A98 +
CW3A98) * (10 ** -6)) + MF1 * ((CF1A1 + CF2A1 + CF3A1) * (10 ** -6)))
m.Equation(MW1 * hW1 + q1 + q2 + q3 + qH1 + qH2 + qH3 + qMED == MW98 * hW98 + MF1 *
418.892 + qC1 + qC2 + qC3 + qLoss)
```

```
m.Equation(qTotal == q1 + q2 + q3)

m.Equation(qCTotal == qC1 + qC2 + qC3)



m.Equation(hW19 == 4.1886652015 * TW19 + 0.0259362067)
m.Equation(hW20 == 4.1886652015 * TW20 + 0.0259362067)
m.Equation(hW21 == 4.1886652015 * TW21 + 0.0259362067)

m.Equation(hW19A == 4.1886652015 * TW19A + 0.0259362067)
m.Equation(hW20A == 4.1886652015 * TW20A + 0.0259362067)
m.Equation(hW21A == 4.1886652015 * TW21A + 0.0259362067)



m.Equation(hW25 == 4.1886652015 * TW25 + 0.0259362067)
m.Equation(hW26 == 4.1886652015 * TW26 + 0.0259362067)
m.Equation(hW27 == 4.1886652015 * TW27 + 0.0259362067)
m.Equation(hW28 == 4.1886652015 * TW28 + 0.0259362067)
m.Equation(hW29 == 4.1886652015 * TW29 + 0.0259362067)
m.Equation(hW30 == 4.1886652015 * TW30 + 0.0259362067)
m.Equation(hW31 == 4.1886652015 * TW31 + 0.0259362067)
m.Equation(hW32 == 4.1886652015 * TW32 + 0.0259362067)
m.Equation(hW33 == 4.1886652015 * TW33 + 0.0259362067)


m.Equation(hW64 == 4.1886652015 * TW64 + 0.0259362067)
m.Equation(hW65 == 4.1886652015 * TW65 + 0.0259362067)
m.Equation(hW66 == 4.1886652015 * TW66 + 0.0259362067)
m.Equation(hW67 == 4.1886652015 * TW67 + 0.0259362067)

m.Equation(hW67MED == 4.1886652015 * TW67MED + 0.0259362067)


m.Equation(hW82 == 4.1886652015 * TW82 + 0.0259362067)
m.Equation(hW83 == 4.1886652015 * TW83 + 0.0259362067)
m.Equation(hW84 == 4.1886652015 * TW84 + 0.0259362067)



m.Equation(hW85 == 4.1886652015 * TW85 + 0.0259362067)
m.Equation(hW86 == 4.1886652015 * TW86 + 0.0259362067)
m.Equation(hW87 == 4.1886652015 * TW87 + 0.0259362067)
m.Equation(hW88 == 4.1886652015 * TW88 + 0.0259362067)
m.Equation(hW89 == 4.1886652015 * TW89 + 0.0259362067)
m.Equation(hW90 == 4.1886652015 * TW90 + 0.0259362067)
m.Equation(hW91 == 4.1886652015 * TW91 + 0.0259362067)
m.Equation(hW92 == 4.1886652015 * TW92 + 0.0259362067)
m.Equation(hW93 == 4.1886652015 * TW93 + 0.0259362067)
m.Equation(hW94 == 4.1886652015 * TW94 + 0.0259362067)
m.Equation(hW95 == 4.1886652015 * TW95 + 0.0259362067)
m.Equation(hW96 == 4.1886652015 * TW96 + 0.0259362067)
m.Equation(hW97 == 4.1886652015 * TW97 + 0.0259362067)



#################################################################################

m.Equation(MAir10 == MAir1 + MAir1Out)
m.Equation(MAir20 == MAir2 + MAir2Out)

m.Equation(MAir == MAir1 + MAir2)



m.Equation(MAir == MAirMED + MAirOut)

m.Equation(MAir1 * hAir1 + MAir2 * hAir2 == MAir * hAir)
```

```
m.Equation(qMED == MAirMED * (hAir - hAirMEDOut))

m.Equation(MW67MEDV1 * (hW67MED1 - 418.892) == MAirMED * (hAir - hAirMEDInt))




m.Equation(MAirOut == MAirOut1 + MAirOut2 + MAirOut3)

m.Equation(MAirOut1 + MAirOut2 + MAirOut3 + MAirMED == MAirOutOut)
m.Equation(MAirOut1 * hAirOut1 + MAirOut2 * hAirOut2 + MAirOut3 * hAirOut3 + MAirMED *
hAirMEDOut == MAirOutOut * hAirOutOut)


m.Equation(MAirOut1 * (hAir - hAirOut1) == qH1)
m.Equation(MAirOut2 * (hAir - hAirOut2) == qH2)
m.Equation(MAirOut3 * (hAir - hAirOut3) == qH3)


m.Equation(hAir == 1.0700 * TAir + 265.1454)
m.Equation(hAirMEDInt == 1.0700 * TAirMEDInt + 265.1454)
m.Equation(hAirMEDOut == 1.0700 * TAirMEDOut + 265.1454)


m.Equation(hAirOut1 == 1.0700 * TAirOut1 + 265.1454)
m.Equation(hAirOut2 == 1.0700 * TAirOut2 + 265.1454)
m.Equation(hAirOut3 == 1.0700 * TAirOut3 + 265.1454)
m.Equation(hAirOutOut == 1.0700 * TAirOutOut + 265.1454)


################################################################################


# Objective-Function (Minimization of Total Annualized Costs)

m.Obj(1.8499 * (MW1 / 999) + (23.66e-6) * qTotal + (0.1459 * (1 / 0.95) * (1 / 3600)) *
qCTotal) # Objective


m.solve() # Solve
```

A7. Case-study 2 Optimisation Model for the Thermal Process System (Modelica code)

The DP model developed for case-study 2 is presented in Code Listing A3. The association of the defined variables to each stream and WEIS component for case-study 2 is presented in Figure A6 (in which each stream/ component within the WEIS flow sheet is characterized according to its definition in the developed code).

Code Listing A3. Optimisation model for the thermal process system of case-study 2 (Modelica code)

```
model CS2TP5
    extends Modelica.Icons.Example;
  // Decision Variables
  //
  //  Thermal Process System
  //
  //
  //
  Real M1(min = 0.00, max = 127.50);
  Real M2(start = 24952.00, min = 0.00, max = 24952.00) annotation(isConstraint =
true);
  Real M2A(start = 24952.00, min = 0.00, max = 24952.00) annotation(isConstraint =
true);
  Real M3(start = 25079.50, min = 0.00, max = 25079.50) annotation(isConstraint =
true);
  Real M4 = 21622.10;
  Real M5 = 21622.10;
  input Real M6(start = 1000.00, min = 0.00, max = 21622.10);
  Real M6A(start = 1000, min = 0.00, max = 21622.10) annotation(isConstraint = true);
  Real M6AA;
  Real M7 = 6141.2398372;
  Real M8(min = 0.00, max = 120.10);
  Real M9(start = 30736.00, min = 0.00, max = 30736.00) annotation(isConstraint =
true);
  Real M9A(start = 30736.00, min = 0.00, max = 30736.00) annotation(isConstraint =
true);
  Real M10(start = 30856.1, min = 0.00, max = 30856.1) annotation(isConstraint = true);
  Real M11 = 16528.40;
  Real M12 = 16528.40;
  input Real M13(start = 4800, min = 0.00, max = 16528.40);
  Real M13A(start = 1000, min = 0.00, max = 16528.40) annotation(isConstraint = true);
  Real M13AA;
  Real M14 = 0.00;
  Real M15(start = 30856.1, min = 0.00, max = 30856.1) annotation(isConstraint = true);
  Real M16(start = 94086.1, min = 0.00, max = 94086.1) annotation(isConstraint = true);
  Real M17(start = 94086.1, min = 0.00, max = 94086.1) annotation(isConstraint = true);
  Real M18(min = 0.00, max = 20.26);
  Real M19(start = 7832.74, min = 0.00, max = 7832.74) annotation(isConstraint = true);
  Real M20(start = 7853.00, min = 0.00, max = 7853.00) annotation(isConstraint = true);
  Real M21(min = 0.00, max = 76.73);
  Real M22(start = 14629.30, min = 0.00, max = 14629.30) annotation(isConstraint =
true);
  Real M23(start = 14706.00, min = 0.00, max = 14706.00) annotation(isConstraint =
true);
  Real M24(start = 30856.1, min = 0.00, max = 30856.1) annotation(isConstraint = true);
  Real M25(start = 30856.1, min = 0.00, max = 30856.1) annotation(isConstraint = true);
  Real M26(start = 78150.04, min = 0.00, max = 78150.04) annotation(isConstraint =
true);
  Real M27(start = 78150.04, min = 0.00, max = 78150.04) annotation(isConstraint =
true);
  //
  //
  //
  Real AF1 = 195.701960784;
  Real AF2 = 255.920066611;
  Real AF3 = 386.611056269;
  Real AF4 = 190.659455233;
  //
  //
  //
```

```
  Real T1 = 34.0;
  Real T2(start = 41.5, min = 41.5, max = 300) annotation(isConstraint = true);
  Real T2A(start = 41.5, min = 41.5, max = 300) annotation(isConstraint = true);
  Real T3(start = 104.7, min = 104.7) annotation(isConstraint = true);
  Real T4 = 41.5;
  Real T5 = 111.5;
  Real T6 = 111.5;
  Real T6A = 111.5;
  Real T6AA = 111.5;
  Real T7 = 111.5;
  Real T8 = 34.0;
  Real T9(start = 41.5, min = 41.5, max = 300) annotation(isConstraint = true);
  Real T9A(start = 41.5, min = 41.5, max = 300) annotation(isConstraint = true);
  Real T10(start = 84.2, min = 84.2) annotation(isConstraint = true);
  Real T11 = 41.5;
  Real T12 = 196.5;
  Real T13 = 196.5;
  Real T13A = 196.5;
  Real T13AA = 196.5;
  Real T14 = 196.5;
  Real T15(start = 196.5, min = 111.5, max = 196.5) annotation(isConstraint = true);
  Real T16(start = 196.5, min = 84.2, max = 196.5) annotation(isConstraint = true);
  input Real T17(min = 70, max = 196.5);
  Real T18 = 35.0;
  Real T19(start = 41.5, min = 41.5, max = 300) annotation(isConstraint = true);
  Real T20 = 59.1;
  Real T21 = 35.0;
  Real T22(start = 41.5, min = 41.5, max = 300) annotation(isConstraint = true);
  Real T23 = 127.1;
  Real T24(start = 196.5, min = 111.5, max = 196.5) annotation(isConstraint = true);
  Real T25(start = 41.5, min = 41.5, max = 196.5) annotation(isConstraint = true);
  Real T26 = 41.5;
  Real T27(start = 41.5, min = 41.5, max = 196.5) annotation(isConstraint = true);
  //
  //
  //
  Real T28 = 84.534472817;
  //
  //
  //
  Real h1 = 0.00;
  Real h2(start = 309.5504, min = 309.5504, max = 586.1454) annotation(isConstraint =
true);
  Real h2A(start = 309.5504, min = 309.5504, max = 586.1454) annotation(isConstraint =
true);
  Real h3(start = 377.1744, min = 377.1744) annotation(isConstraint = true);
  Real h4 = 309.5504;
  Real h5 = 384.4504;
  Real h6 = 384.4504;
  Real h6A = 384.4504;
  Real h6AA = 384.4504;
  Real h7 = 384.4504;
  Real h8 = 0.00;
  Real h9(start = 309.5504, min = 309.5504, max = 586.1454) annotation(isConstraint =
true);
  Real h9A(start = 309.5504, min = 309.5504, max = 586.1454) annotation(isConstraint =
true);
  Real h10(start = 355.2394, min = 355.2394) annotation(isConstraint = true);
  Real h11 = 309.5504;
  Real h12 = 475.4004;
  Real h13 = 475.4004;
  Real h13A = 475.4004;
  Real h13AA = 475.4004;
  Real h14 = 475.4004;
  Real h15(start = 475.4004, min = 384.4504, max = 475.4004) annotation(isConstraint =
true);
  Real h16(start = 475.4004, min = 355.2394, max = 475.4004) annotation(isConstraint =
true);
  Real h17(min = 340.0454, max = 475.4004) annotation(isConstraint = true);
  Real h18 = 0.00;
  Real h19(start = 309.5504, min = 309.5504, max = 586.1454) annotation(isConstraint =
true);
  Real h20 = 328.3824;
  Real h21 = 0.00;
  Real h22(start = 309.5504, min = 309.5504, max = 586.1454) annotation(isConstraint =
true);
  Real h23 = 401.1424;
```

```
  Real h24(start = 475.4004, min = 384.4504, max = 475.4004) annotation(isConstraint =
true);
  Real h25(start = 309.5504, min = 309.5504, max = 475.4004) annotation(isConstraint =
true);
  Real h26 = 309.5504;
  Real h27(start = 309.5504, min = 309.5504, max = 475.4004) annotation(isConstraint =
true);
  //
  //
  //
  Real h28 = 355.59728591;
  //
  //
  //
  Real MPCM() annotation(isConstraint = true);
  Real CPPCM();
  //
  //
  //
  Real L = 10;
  Real rint = 0.10;
  Real rext = 0.12;
  //
  //
  //
  Real TPCM(start = 41.5, min = 41.5, max = 196.5) annotation(isConstraint = true);
  Real TPCM1(start = 196.5, min = 41.5, max = 196.5) annotation(isConstraint = true);
  Real TPCMN(start = 196.5, min = 41.5, max = 196.5) annotation(isConstraint = true);
  //
  //
  //
  Real Elec(min = (262.35867551 * (1 / 999) * 2.5)) annotation(isConstraint = true);
  //
  //
  //
  Real OBJ;
  Real OBJEff(start = 0, fixed = true) annotation(isMayer = true);
  //
  //Real OBJ1;
  //Real OBJEff1;
  //
  // Parameters
  //
  Real ORCEfficiency = 1.50;
  //
  //
  //
equation
//
//
//
  if time <= 1e-60 then
    M6AA = 10000;
    M13AA = 10000;
  else
    M6AA = 12000;
    M13AA = 10000;
  end if;
//
// Constraints
//
  M2 + M6AA = M2A;
  M2 * h2 + M6AA * h6AA = M2A * h2A;

  M2A = AF1 * M1;

  M1 + M2A = M3;
  M1 * (h1 + (45.1e3)) + M2A * h2A + (25079.50 * 1.05 * (104.7 - 253.1802139)) = M3 *
h3;


  127.50 * (45.1e3) = M1 * (45.1e3) + M2A * (h2A - 309.5504);



  M5 = M6 + M6A + M6AA + M7;
```

```
  M9 + M13AA = M9A;
  M9 * h9 + M13AA * h13AA = M9A * h9A;


  M9A = AF2 * M8;

  M8 + M9A = M10;
  M8 * (h8 + (45.1e3)) + M9A * h9A + (30856.1 * 1.05 * (84.2 - 209.3276856)) = M10 *
h10;


  120.10 * (45.1e3) = M8 * (45.1e3) + M9A * (h9A - 309.5504);


  M12 = M13 + M13A + M13AA + M14;


  M6 + M13 = M24;
  M6 * h6 + M13 * h13 = M24 * h24;


  M7 + M14 = M15;
  M7 * h7 + M14 * h14 = M15 * h15;

  M6A + M13A + M3 + M10 + M7 + M14 = M16;
  M6A * h6A + M13A * h13A + M3 * h3 + M10 * h10 + (M7 + M14) * h28 = M16 * h16;

  M16 = M17;
  M16 * (h16 - h17) * (ORCEfficiency * 0.01) = Elec * 3600;



  M19 = AF3 * M18;

  M18 + M19 = M20;


  if time <= 25.5 * 3600 then
    M19 = 1e-60;
  else
    20.26 * (45.1e3) = M18 * (45.1e3) + M19 * (h19 - 309.5504);
  end if;




  M22 = AF4 * M21;

  M21 + M22 = M23;


  if time <= 25.5 * 3600 then
    M21 = 1e-60;
  else
    76.73 * (45.1e3) = M21 * (45.1e3) + M22 * (h22 - 309.5504);
  end if;




  M24 = M25;
  if time <= 25.5 * 3600 then
    M24 * (h24 - h25) * (1000 / 3600) = MPCM * CPPCM * der(TPCM);
  else
    M24 * (h24 - h25) * (1000 / 3600) = 0;
  end if;

  M26 = M27;
  if time <= 25.5 * 3600 then
    M26 * (h26 - h27) * (1000 / 3600) = 0;
  else
    M26 * (h26 - h27) * (1000 / 3600) = MPCM * CPPCM * der(TPCM);
  end if;
```

```
  M27 = M2 + M9 + M19 + M22;
  h27 = h2;
  h27 = h9;
  h27 = h19;
  h27 = h22;

  CPPCM = 225000 / ((2 * 3.1416) ^ 0.5 * 0.1626) * exp(-(TPCM - 72) ^ 2 / (2 * 0.1626 ^
2)) + 2200;

  if time <= 25.5 * 3600 then
    TPCM1 = ((T24 + T25) * 0.5);
    TPCMN - ((T24 + T25) * 0.5) = (41.5 - ((T24 + T25) * 0.5)) * (-1 + (2 / (1 + exp(-
2.5 * (rext / (2 * (((0.15 / (890 * 2200)) * (time + (1e-60))) ^ 0.5)))))));
  else
    TPCM1 - ((T26 + T27) * 0.5) = (196.5 - ((T26 + T27) * 0.5)) * (-1 + (2 / (1 + exp(-
2.5 * ((0.001) / (2 * (((0.15 / (890 * 2200)) * (time + (1e-60))) ^ 0.5)))))));
    TPCMN = ((T26 + T27) * 0.5);
  end if;
  MPCM = 120 * 890 * (L * 3.1416 * ((rext ^ 2) - (rint ^ 2)));
//
//
//
  h2 = 1.0700 * T2 + 265.1454;
h2A = 1.0700 * T2A + 265.1454;
h3     = 1.0700 * T3 + 265.1454;
h9     = 1.0700 * T9 + 265.1454;
h9A    = 1.0700 * T9A + 265.1454;
h10    = 1.0700 * T10 + 265.1454;
h15    = 1.0700 * T15+ 265.1454;
h16    = 1.0700 * T16 + 265.1454;
h17    = 1.0700 * T17 + 265.1454;
h19    = 1.0700 * T19 + 265.1454;
h22    = 1.0700 * T22 + 265.1454;
h24    = 1.0700 * T24 + 265.1454;
h25    = 1.0700 * T25 + 265.1454;
h27    = 1.0700 * T27 + 265.1454;
//
//
//
  if time <= 25.5 * 3600 then
    der(TPCM) = 0.15 / (890 * CPPCM) * (1 / ((rext + rint) * 0.5) * ((TPCMN - TPCM1) /
(rext - rint) + (TPCMN - 2 * TPCM + TPCM1) / (rext - rint) ^ 2));
  else
    der(TPCM) = 0.15 / (890 * CPPCM) * (1 / ((rext + rint) * 0.5) * ((TPCM1 - TPCMN) /
(rext - rint) + (TPCM1 - 2 * TPCM + TPCMN) / (rext - rint) ^ 2));
  end if;
//
//
//
  OBJ = (23.66 * 0.0451 * (M1 + M8 + M18 + M21) + 0.1459 * (-(Elec - 262.35867551 * (1
/ 999) * 2.5))) * (1 / 3600);
  der(OBJEff) = OBJ;
//
//
//
  annotation(
    experiment(StartTime = 0, StopTime = 151200, Tolerance = 1e-07, Interval = 756),
    __OpenModelica_simulationFlags(s = "optimization", optimizerNP = "3"),
    __OpenModelica_commandLineOptions = "+g=Optimica");
end CS2TP5;
```

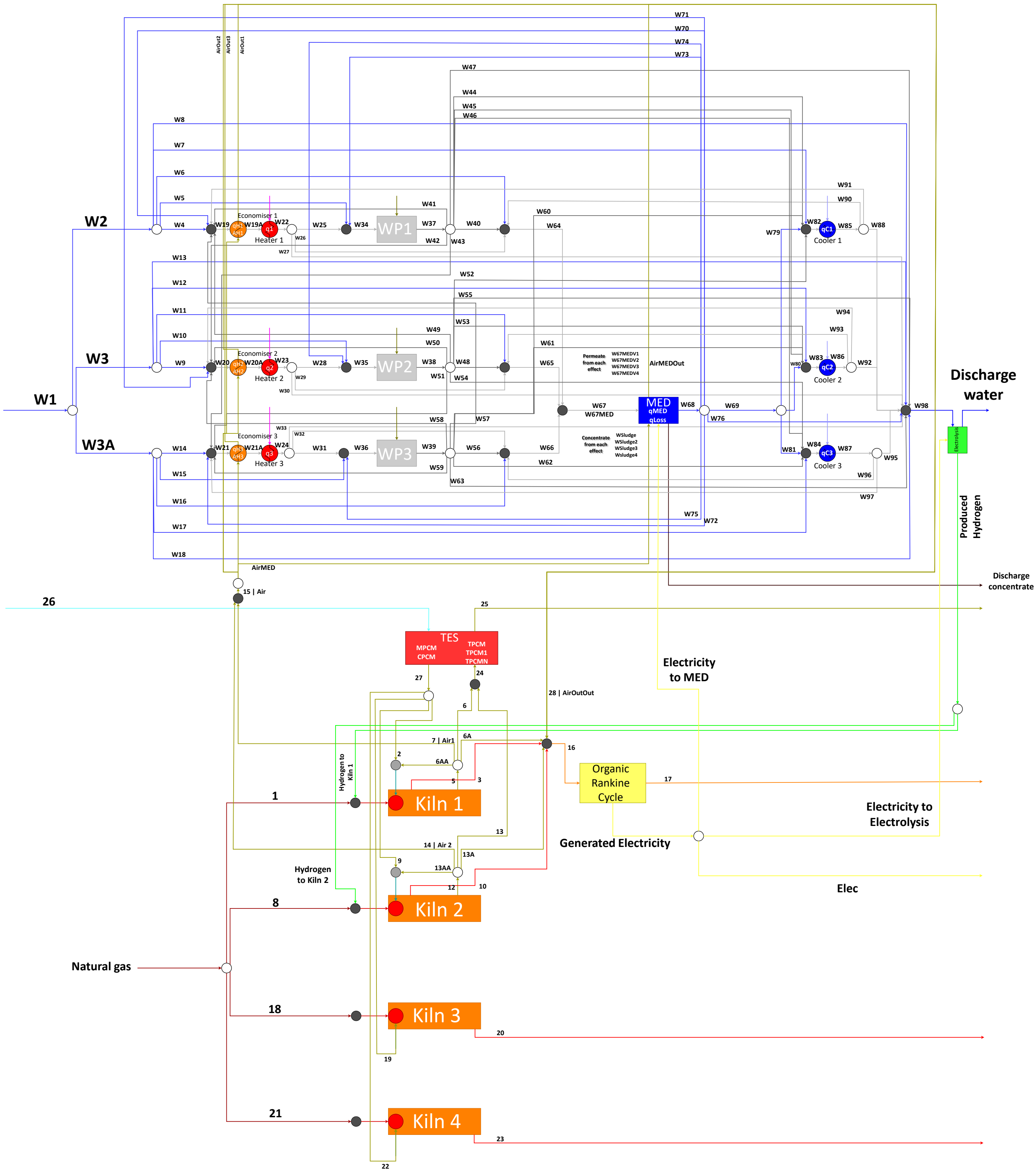

Figure A6. Flowsheet for the Case-study 2 WEIS including the stream and sizing parameters references considered in the scripting of the optimisation models Python and Modelica codes

A8. Determination of the Investment Cost associated to WEIS Projects

In Table A4, the formulas for the estimation of the base cost associated to each component of the conceptualized WEIS are presented. In Table A5, the determination method used to calculate direct and indirect costs parcels associated to the WEIS projects are presented.

Table A4. Estimation formulas for the base cost associated to each component of the conceptualized WEIS

Component	Key Design parameter	Base Cost Calculation Formula
Heat Exchangers (Economisers, Air preheaters and PCM-based heat exchanger)	Heat Transfer Area ($\mathrm{A_{HT}}$)	$\mathrm{CAPEX_{Comp.}(€) = 1578.24 \cdot A_{HT}\ (m^2)^{0.81}}$
Organic Rankine Cycle (ORC)	Nominal Generated Power ($\mathrm{Pot_{nom}}$)	$\mathrm{CAPEX_{Comp.}(€) = (2.345 \cdot 10^6) \cdot \frac{Pot_{nom}(W)}{1115}^{0.86}}$
Multi-effect distillation (MED)	Produced treated water ($\mathrm{M_{TW}}$)	$\mathrm{CAPEX_{Comp.}(€) = 2535 \cdot \left(\frac{M_{TW}\ (kg/h)}{999\ (kg/m^3)} \cdot 24\ (h/day)\right)^{0.9751}}$

Table A5. Characterization of the primarily considered fluids

Component	Share over Cost	Definition	Association to WEIS Component and Aspect
Heat Exchangers (Economisers, Air preheaters and PCM-based heat exchanger)	45% of base cost	Base equipment assembly	
	10% of base cost	Thermal insulation	Thermal insulation of heat exchangers
	30% of base cost	Supervision	
	30% of base cost	Undertaking	
	20% of base cost	Provision for contingencies	
Organic Rankine Cycle (ORC)	45% of base cost	Base equipment assembly	
	65% of base cost	Pipes	Pipes for the passage of organic fluid and ducts for the passage of hot air and exhaust gases.
	80% of base cost	Utilities and services	System-wide utilities, such as the organic working fluid (NOVEC649).
	30% of base cost	Control	Installation of process control equipment (such as sensors).
	15% of base cost	Electric installations	Installation of equipment for electric power generation and transmission from the ORC system.
	10% of base cost	Thermal insulation	Thermal insulation of the

			components of the ORC system.
	30% of base cost	Supervision	
	30% of base cost	Undertaking	
	20% of direct and indirect costs	Provision for contingencies	
Multi-effect distillation (MED)	45% of base cost	Base equipment assembly	
	65% of base cost	Pipes	Pipes installed around the whole water system.
	30% of base cost	Control	Installation of process control equipment (such as sensors) around the water system.
	15% of base cost	Electric installations	Installation of electric power transmission system to centrifugal pumps.
	10% of base cost	Thermal insulation	Thermal insulation of pipes installed around the water system.
	30% of base cost	Supervision	
	30% of base cost	Undertaking	
	20% of direct and indirect costs	Provision for contingencies	

A9. Unitary prices and Emissions factors associated to energy and water utilities

In Table A6, the values for unitary prices and emission factors associated to each energy and water use utility are presented.

Table A6. Unitary prices and emission factor associated to the energy and water utilities considered in the approached case-studies

Utility	Unitary Price	Equivalent Carbon Dioxide Emission Factor
Natural gas	23.66 €/GJ	64.1 kg $CO_{2,eq}$/GJ
Electricity	0.1459 €/kWh	0.47 kg $CO_{2,eq}$/kWh
Water system hot utility (natural gas)	23.66 €/GJ	64.1 kg $CO_{2,eq}$/GJ
Water system cold utility (electricity)	0.1459 €/kWh	0.47 kg $CO_{2,eq}$/kWh
Water	1.8499 €/m^3	

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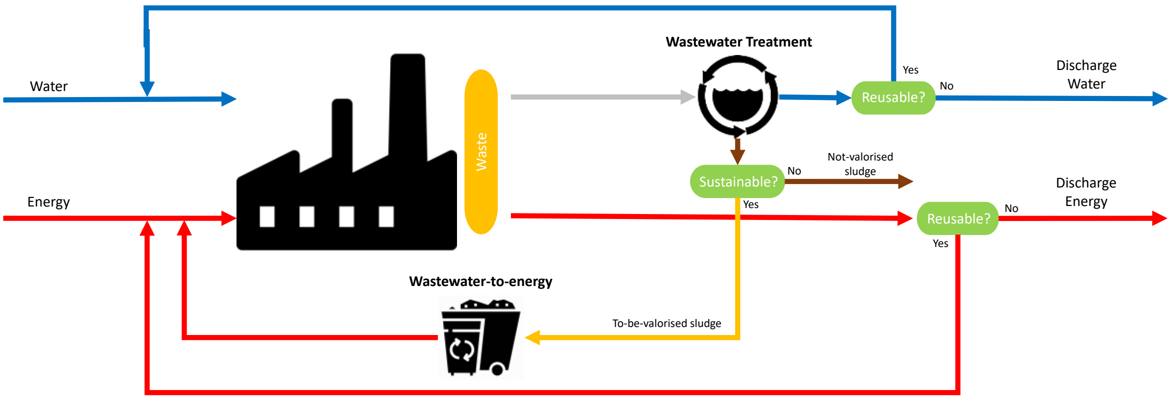

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