DEVELOPMENT OF STRATEGIES FOR WASTE VALORISATION IN WASTE WATER TREATMENT PLANTS (WWTPS): CONSORCI BESÒS TORDERA CASE STUDY

David Palma Heredia

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Universitat de Girona

DOCTORAL THESIS

Development of strategies for waste valorisation in Waste Water Treatment Plants (WWTPs): Consorci Besòs Tordera case study

David Palma Heredia

2020

Universitat de Girona

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2020

DOCTORAL PROGRAMME IN WATER SCIENCE AND TECHNOLOGY

Supervisors: Dr. Manel Poch Espallargas, Dr. Miquel Àngel Cugueró Escofet

Tutor: Dr. Manel Poch Espallargas

PhD thesis submitted to aim for PhD degree for the University of Girona

List of publications

Indexed scientific journals:

1. D. Palma-Heredia, M. Poch, M.À. Cugueró-Escofet. Implementation of a Decision Support System for Sewage Sludge Management. Sustainability 2020, 12(21), 9089; https://doi.org/10.3390/su12219089

2. D. Palma-Heredia, M. Verdaguer, M. Molinos-Senante, M. Poch, M.À. Cugueró-Escofet Optimised blending for anaerobic co-digestion using ant colony approach: Besòs river basin case study (submitted to the journal Renewable Energy)

International congress publications:

1. D. Palma-Heredia, M. Verdaguer, M. Poch, M. À. Cugueró-Escofet, 'blend quality and logistics optimisation of anaerobic co-digestion in a real multi-plant case study', in International Water Association Resource Recovery 2019 Congress (Venice, Italy)

2. D. Palma-Heredia, M. Poch, M. À. Cugueró-Escofet, 'Feasibility of raw operators' data by uncertainty propagation on elemental mass-balances of Waste Water Treatment Plants', in Watermatex 2019 Congress (Copenhagen, Denmark)

National congress publications:

1. D. Palma-Heredia, M. À. Cugueró-Escofet, M. Poch, and P. Aguiló-Martòs, 'Assessment of WWTP sludge management strategies using a key performance index simulator', in Young Water Professionals 2019 Congress (Madrid, Spain)

2. D. Palma-Heredia, M. Verdaguer, M. Poch, M. À. Cugueró-Escofet, 'Aplicación de algoritmo Ant Colony Optimisation para optimizar estrategias de codigestión centralizada', in VIII Jornada Lodos UB (Barcelona, Spain)

List of abbreviations and symbols

ACO	Ant Colony Optimisation
AD	Anaerobic Digestion
Alk	Alkalinity
BC	Biogas cogeneration
BOD	Biochemical Oxygen Demand
BU	Biogas upgrading
C	Carbon
C1 – C5	Carbon mass balance flows
CBT	Consorci Besòs Tordera
CH4	Methane
Co1 – Co7	External cosubstrate generators
CO2	Carbon dioxide
COD	Chemical Oxygen Demand
CSD	Conventional sludge drying
CTD	Conventional thermal valorisation
DSS	Decision Support System
EPA	Environmental Protection Agency
GHG	Greenhouse Gases
GR	Granollers
HRAS	High Rate Activate Sludge
HRT	Hydraulic retention time
ISO	International Organisation for Standardization
KPI	Key Performance Index
Max-Min	Maximum-Minimum
N	Nitrogen
N1 – N4	Nitrogen mass balance flows

NH4+	Ammonia
NPV	Net Present Value
P	Phosphorous
P	Biogas pressure
PLC	Programmable Logic Controller
PSS	Product Service System
PWM	Plant Wide Model
R	Ideal gas constant
RdM	Re-Distributed Manufacturing
SM	Solid Matter
ST	Single anaerobic treatment
SVM	Solid Volatile Matter
SWOT	Strength – Weakness – Opportunities – Threats
T	Biogas temperature
TH	Thermal hydrolysis
TN	Total Nitrogen
Tox	Toxicity
TSS	Total Suspended Solids
UASB	Upflow Anaerobic Sludge Blanket
W1-W12	Undigested sewage sludge generating WWTPs
WEF nexus	Water-Energy-Food nexus
WRRF	Water Resource Recovery Facility
WWTP	Waste Water Treatment Plant

List of figures

List of tables

Certificate of thesis direction

El Dr. Manel Poch Espallargas del Laboratori d'Enginyeria Química i Ambiental (LEQUIA) de la Universitat de Girona, i el Dr. Miquel Àngel Cugueró Escofet, del Advanced Control Systems Research Group de la Universitat Politècnica de Catalunya

DECLAREM:

Que el treball titulat "Development of strategies for waste valorisation in Waste Water Treatment Plants (WWTPs): Consorci Besòs Tordera case study", que presenta en David Palma Heredia per a l'obtenció del títol de doctor, ha estat realitzat sota la nostra direcció, i que compleix els requisits per poder optar a Menció Industrial.

I perquè així consti i tingui els efectes oportuns, signem aquest document.

Dr. Manel Poch Espallargas   Dr. Miquel Àngel Cugueró Escofet

Girona, de 2020

Agraïments / Agradecimientos / Acknowledgements

Les tesis doctorals són autèntics reptes que poden posar a prova les aptituds dels doctorands. El suport tant directe com indirecte de moltes persones té una influència significativa en el rendiment del projecte. A continuació unes (breus) línies per reconèixer el suport de tanta gent.

En primer lloc, als meus directors de tesi Manel Poch i Miquel Àngel Cugueró. Ells m'han guiat pel millor camí possible, amb les millors orientacions possibles, i m'han ofert un suport continu i una relació immillorable. Des de proveir consell, a revisar ingents quantitats de documents elaborats per mi mateix, passant per la paciència d'iterar i verificar resultats i en especial per la perspectiva que m'han permès aconseguir sobre els diferents mètodes i les bones pràctiques en els processos d'implementació i en les relacions amb àmbits professionals com el sanejament. Gràcies al seu esforç he pogut esdevenir un pont (més o menys sòlid) entre el món de l'acadèmia i el món de la indústria.

També al meu grup de recerca, el LEQUIA. Malgrat no hagi pogut relacionar-me tant com m'hauria agradat (deixant de banda la situació de la pandèmia actual), recordaré els moments que hem tingut: tant si són doctorands, personal investigador o personal administratiu; i tant si ens hem trobat als despatxos, als passadissos (o al bar) de la Facultat de Ciències o en algunes de les diferents trobades fora la universitat. Sou tot un exemple de com han de ser les persones en l'àmbit acadèmic. En especial agrair a la Marta Verdaguer i l'Adrià Riu per la seva paciència i coneixement, que han col·laborat de forma decisiva a fer possible una part d'aquesta tesi.

Com es tracta d'una tesi industrial, tampoc falten els agraïments (i no pocs) a totes aquelles persones professionals que m'han acollit durant aquests anys en el Consorci Besós Tordera i a CCB Serveis Mediambientals, i del que m'han fet partícip de les seves activitats: Josep, Jackson, Francesc, Berta, Andrea, Iván, Francesc (un altre), Begoña, Pere, Albert, Nico, Estela, Espe, Alba, Rosa, Jesús, Mikel, Jose Antonio, Jordi, David, Manel i moltíssima més gent amb la que m'hauria agradat poder relacionar-me i col·laborar; incloent també la gran quantitat de professionals que he conegut a les diverses EDAR que he visitat: com Beatriz, Mónica, Marta, Sonia, Meritxell, Antonio, David, Barbara, Manuel i moltíssims altres professionals de l'àmbit del sanejament que en algun moment o altre m'han ajudat a entendre les particularitats de cada depuradora. L'experiència i aptituds que he adquirit amb totes aquestes persones és un dels regals que més valoraré d'aquests anys de tesi.

També cal reconèixer que ningú és res sense un ambient de vida sa. Com la qualitat de vida del mediterrani (malgrat la multitud de crisis creixents arreu del món), o la relativament bona conservació del medi ambient a Catalunya i a la província de Girona (amb especial menció als meravellosos paisatges del Montseny, que han acompanyat durant molt de temps els meus viatges al Consorci). Però també cal reconèixer que el món és global, i que no som res sense un entreteniment de qualitat per divergir la ment en els moments de major (i menor) esgotament: comunitats d'internet amb relatius desconeguts però amb certes aficions compartides (les famoses "relacions parasocials"); artistes de tota mena (en especial de les arts musicals, però també de les arts visuals o de les arts dramàtiques); i, en general, la gran quantitat de contingut creatiu i inspirador que es pot trobar a internet (si es busca bé).

Per últim, però no per això menys important, els meus profunds agraïments a les amistats (algunes velles, moltes noves) que m'han seguit en aficions recents com els jocs de rol (*Dungeons & Dragons*, bàsicament). I, en especial, a la meva família: per proveir-me d'un ambient educatiu sà, menjar de qualitat, uns valors dignes i progressistes, i de la llibertat de decisió junt amb un suport immens al llarg de la meva vida. En algun moment pot haver-hi diferències, però la nostre maduresa ens permet sortir endavant.

Desitjo que la vida us sigui propícia, i que mai perdeu l'esperança

A vosaltres, moltíssimes gràcies per tot

This thesis was financially supported supported by DAM (Depuración de Aguas del Mediterráneo) and by the Industrial Doctorate Programme (ref. 2017-DI-048) of the Catalan Agency of University and Research Grants Management (AGAUR). LEQUIA has been recognized as a consolidated research group by the Catalan Government with code 2014-SGR-1168. The author would also like to acknowledge the support received from his colleagues: Adrià Riu of the Laboratory of Chemical and Environmental Engineering (LEQUIA) of the University of Girona (UdG) for his programming expertise and Pere Aguiló and Begoña Martínez of *Consorci Besòs Tordera* (CBT) for their useful comments and insights about the anaerobic digestion and other sewage sludge treatment processes involved in this work.

Resum

La sostenibilitat és un concepte ideal amb una tendència al alça entre tots els sectors d'activitat de la societat humana, tots ells moguts per la mateixa motivació: l'existència d'una crisi global de recursos, que afecta múltiples sectors de l'activitat humana i pot significar una pèrdua potencial de qualitat de vida de la humanitat. Una via ben coneguda per intentar aconseguir un major grau de sostenibilitat és l'aplicació del canvi de paradigma d'economia lineal a circular, la qual permet reduir els residus produïts i incrementar els recursos disponibles simultàniament.

Ja que l'aigua és un dels recursos més essencials, el sistema de sanejament del cicle urbà de l'aigua és un sector estratègic prominent on la implementació de l'economia circular s'hi pot dur a terme. Les estacions depuradores d'aigua residual (EDAR), com a nexe aigua-energia-alimentació, poden proveir de diferents recursos recuperables, com aigua potable, energia i nutrients a través de les tecnologies sostenibles. Tot i això, l'adequada planificació del desenvolupament de les EDAR, incloent diferents tecnologies sostenibles, és una preocupació creixent degut a la complexitat de tal tasca i al context de ràpids canvis de la societat moderna.

L'objectiu de la tesi és el desenvolupament i aplicació a un cas d'estudi real d'un mètode que permeti facilitar la planificació de desenvolupament de les EDAR i la implementació de processos relatius a l'economia circular en l'àmbit del sector del tractament d'aigües residuals. En el sistema de l'EDAR, el fang de depuració és el principal residu produït. Per tant, els processos relatius a la producció, transformació i valorització d'aquest són el focus de la tesi.

Com es detalla al Capítol 3, els mètodes aplicats estan basats en els conceptes d'anàlisi de sistemes i desenvolupament de sistemes d'ajut a la decisió (SAD). Així, es seleccionen dos principals estratègies clau d'implementació d'economia circular, i per a cadascuna d'elles es desenvolupen metodologies adaptades que s'apliquen al cas d'estudi com aplicacions d'usuari.

La metodologia és validada per aplicació d'aquesta a un cas d'estudi real, que comprèn un entorn heterogeni amb 26 EDAR, gestionades per l'entitat pública *Consorci Besòs Tordera* (CBT).

En el Capítol 4, un anàlisi exhaustiu de la infraestructura del cas d'estudi i els seus processos associats es duu a terme. Es realitza un exercici comparatiu per avaluar l'eficiència i el potencial del cas d'estudi respecte referents internacionals, amb especial èmfasi en la línia de fangs de depuració.

En els Capítols 5 i 6, les dos estratègies clau seleccionades en el Capítol 3 són desenvolupades i aplicades. D’una banda, es desenvolupa una eina per a la generació d’avaluacions integrals i semiautomàtiques sobre la implementació de nous processos relatius a la valorització de residus (específicament dels fangs de depuració dels sistemes de sanejament); aquest repte es soluciona mitjançant el desenvolupament d’un simulador de processos d’EDAR integrat amb SAD, que utilitza un conjunt d’indicadors de rendiment per a l’avaluació de cada escenari. D’altra banda, s’aborda l’optimització de la digestió anaeròbia i la seva potenciació a través de la co-digestió, combinada amb el tractament centralitzat de fang de depuració no digerit, mitjançant el desenvolupament d’un algoritme d’optimització innovador basat en els mètodes combinatoris de l’algorisme de la colònia de formigues (*Ant-Colony Optimisation*) incloent aspectes relatius a la planificació logística.

Els Capítols 7 i 8 resumeixen una discussió general de les eines desenvolupades, les seves limitacions i els seus impactes potencials i marquen el camí per millorar la planificació de desenvolupament de les EDAR i optimitzar la implementació de l’economia circular.

Resumen

La sostenibilidad es un concepto ideal con una tendencia al alza entre todos los sectores de actividad de la sociedad humana, movidos por la misma motivación: una crisis global de recursos, que afecta múltiples sectores de la actividad humana y que pueden conllevar una pérdida global de la calidad de vida de la humanidad. Una vía bien conocida para intentar conseguir un mayor grado de sostenibilidad es la aplicación del cambio de paradigma de economía lineal a circular, que permite reducir los residuos producidos e incrementar los recursos disponibles simultáneamente.

Dado que el agua es uno de les recursos más esenciales, el sistema de saneamiento del ciclo urbano del agua es un sector estratégico prominente donde la implementación de la economía circular se puede llevar a cabo. Las estaciones depuradoras de agua residual (EDAR), como nexo agua-energía-alimentación, pueden proveer de diferentes recursos recuperables, como agua potable, energía y nutrientes, a través de las tecnologías sostenibles. No obstante, la adecuada planificación del desarrollo de las EDAR, combinada con las tecnologías sostenibles, es una preocupación creciente debido a la complejidad de tal tarea y al contexto de rápidos cambios de la sociedad moderna.

El objetivo de la tesis es desarrollar y aplicar a un caso de estudio real un método que permita facilitar la planificación del desarrollo de EDAR y la implementación de procesos relativos a la economía circular en el sector del saneamiento. En el sistema de la EDAR, el fango de depuración es el principal residuo producido. Por tanto, los procesos relativos a su producción, transformación y valorización son el foco de la tesis.

Como se detalla en el Capítulo 3, los métodos aplicados están basados en los conceptos de análisis de sistemas y desarrollo de sistemas de ayuda a la decisión (SAD). Así, se seleccionan dos principales estrategias clave de implementación de economía circular, y para cada una de ellas se desarrollan metodologías adaptadas que se aplican al caso de estudio como aplicaciones de usuario.

La metodología es validada por medio de su aplicación a un caso de estudio real, que comprende un entorno heterogéneo con 26 EDAR, gestionadas por la entidad pública *Consorci Besòs Tordera* (CBT).

En el Capítulo 4, un análisis exhaustivo de la infraestructura del caso de estudio y sus procesos asociados se lleva a cabo. Se ejecuta un ejercicio de comparación para evaluar la eficiencia y el

potencial del caso de estudio respecto referentes internacionales, con especial énfasis en la línea de fango de depuración.

En los Capítulos 5 y 6, las estrategias clave seleccionadas en el Capítulo 3 son desarrolladas y aplicadas. Por un lado, es desarrolla una herramienta para la generación de evaluaciones integrales y semiautomáticas sobre la implementación de nuevos procesos relacionados con la valorización de residuos (específicamente de los fangos de depuración de los sistemas de saneamiento); este reto se soluciona mediante el desarrollo de un simulador de procesos de EDAR integrado con SAD, que utiliza un set jerárquico de indicadores de rendimiento para evaluar cada escenario. Por otro lado, se aborda la optimización de la digestión anaerobia y su potenciación a través de la co-digestión combinada con el tratamiento centralizado del fango no digerido; esto se aproxima con el desarrollo de un algoritmo de optimización innovador basado en los métodos combinatorios del algoritmo de la colonia de hormigas (*Ant Colony Optimisation*) e incluye aspectos relativos a la planificación logística.

Los Capítulos 7 y 8 resumen una discusión general de las herramientas desarrolladas, sus limitaciones y su impacto esperado y marcan el camino para mejorar la planificación del desarrollo de las EDAR y optimizar la implementación de la economía circular.

Summary

Sustainability is an uprising concept amongst many sectors of activity of the human society, stirred by the same motivation: a global resource crisis that affects multiple sectors of human activity and can potentially mean an overall loss of life quality for humankind. One well known way to try to achieve a higher degree of sustainability is through a paradigm shift from linear to circular economy, which allows reducing waste and increasing available resources simultaneously.

Since water is one the most essential resources, the sanitation system of the urban water cycle is a prominent strategic sector where the implementation of circular economy can be performed. Waste water treatment plants (WWTPs), as a water-energy-food nexus, can provide different recoverable resources, such as clean water, energy and nutrients through different sustainable solutions. However, proper development planning for WWTPs, coupled with such sustainable solutions, is an increasing concern due to the complexity of such task and the rapidly changing environment of the modern society.

The objective of this thesis is to develop and apply to a real case study a method to allow easier WWTP development planning and implementation of circular economy related processes in the wastewater treatment sector. In the WWTP system, sewage sludge is the main waste produced. Hence, the processes regarding its production and transformation are the focus of the thesis.

As detailed in Chapter 3, the applied methods are based on the concepts of system analysis and development of Decision Suport Systems (DSS). Overall, two main key strategies of circular economy implementation are selected, and for each of them adapted methodologies are developed and successfully applied to the case study as end-user tools.

The methodology is validated through its application to a real case study, which comprises a heterogeneous environment with 26 WWTPs, managed by the public entity *Consorci Besòs Tordera* (CBT).

In Chapter 4, a comprehensive analysis of the case study infrastructure and associated processes is performed. A benchmark exercise is executed to assess the efficiency and potential of the case study in regards to international references, with special focus on the sewage sludge line.

In Chapters 5 and 6, the two key strategies selected in Chapter 3 are developed and applied. On the one hand, a tool is developed for the generation of integrated and semiautomatic assessments about the implementation of new processes related to waste valorisation (focused on the sewage sludge of sanitation systems); this challenge is solved through the development of an integrated DSS and WWTP process simulator that uses a hierarchical set of Key Performance Indicators (KPIs) for the evaluation of each scenario. On the other hand, it is tackled the optimisation of anaerobic digestion and enhancement through co-digestion coupled with centralized treatment of non-digested sewage sludge; this is approached by developing an innovative optimisation algorithm based on the combinatorial methods of Ant-Colony Optimisation, which includes logistic planning related issues.

Chapters 7 and 8 summarize a general discussion over the developed toolboxes, their limitations and potential impacts and mark the path for further improvement of WWTP's development planning and optimisation of circular economy implementation.

Table of contents

Chapter One

Introduction

1.1 The global resource crisis and the linear economy

It is a well-proven fact that the increase of population, due to an increase of life quality and the achievement of different scientific milestones, has as a consequence the increase of demand of all sorts of commodities (from food to energy). As a result, to sustain such increasingly human population worldwide, during the last decades the production system has increased as well. However, since the production system depends on resource extraction, an increase of demand is related with an increase of the production, hence an increase of resource extraction.

The key point is that resources are limited to those available within planet Earth. This means that eventually the production system will not be able to meet population demands due to resource scarcity. Actually, this phenomenon has already been observed during the last years with the well-known examples of the fuel or fertilizer industries (which, in turn, are bound to two great population demands such as energy and food, respectively).

Even more, resources are not only limited, but also unequally distributed over the planet. This, together with the fact that humankind is organized through relatively independent countries, each with their own government, military and diplomacy strategies, is one of the greatest sources of human conflicts.

Pollution is another great issue bound to the increase of the production system. Energy is a basic demand, and one of the most common ways to obtain energy has been (and it still is nowadays) by burning fossil fuels. This process produces significant emissions of greenhouse gases (GHG), which contribute to climate change [1].

The aforementioned facts (i.e. limited and unequally distributed resources and pollution from energy production systems) are the main drivers of the present global resource crisis. It affects all sectors of human activity and all sorts of human demands (from the basic ones such as food, energy, health and safety to further “complementary” commodities such as electronic devices).

The global resource crisis is bound to the production system, which is based on linear economy, rather than human “overpopulation” (which is considered an unavoidable process and all attempts at directly addressing often carry heavy ethical burdens). Actually, many economists agree that linear economy production model is the major responsible of the global resource crisis, and also that by improving current production systems the global resource crisis could be attenuated [2].

Production systems based on linear economy are characterised by materials (or resources) flowing in a straight line from resource extraction, manufacturing and disposal (or the “take-make-dispose” steps); also note that energy consumption in the manufacturing step, as well as the disposal step, are responsible for most amounts of pollution. That model has not changed since industrial revolution (and maybe since the dawn of humankind), but no significant changes have been made to prevent its effects. Until the last decades, where, due to human demand increase, resource consumption and environment pollution have reached and surpassed many critical points, putting in danger the biosphere of planet Earth and, hence, the future of humankind [3]. Besides, the only possible way for any production system to achieve “value” within linear economy, according to the axiom of “infinite economic growth”, is through consuming, producing, selling and disposing (and polluting) as much as possible. Figure 1 illustrates how linear economy contributes to an overall degradation of the biosphere.

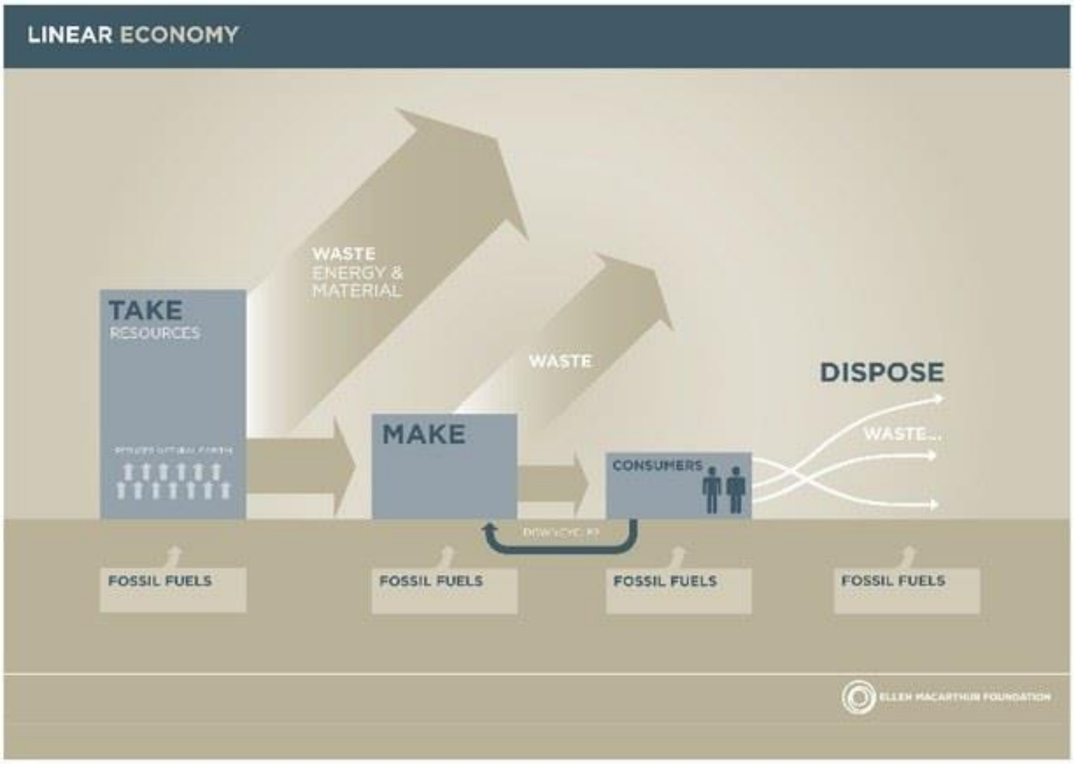

Figure 1. Linear economy overview and impacts. Source: Ellen Macarthur Foundation https://www.ellenmacarthurfoundation.org/news/circular-economy

1.2 The concepts of sustainability and circular economy

A simple definition of sustainability states it as the “ability to exist constantly” [4]. So, sustaining the current human demands with the current production system (linear economy based) is not sustainable, since linear economy production systems are progressively endangering the biosphere, surpassing critical points until eventually provoking the collapse of human civilisation. This self-contradiction is the reason for which a new, more accurate concept of sustainability was designed when referred to the progress of human civilisation: generally, it refers to the capacity for the human civilisation and the biosphere to coexist; more specifically, it refers to keep economy development without provoking detrimental effects upon society or environment. Figure 2 shows how those three “dimensions” of sustainability are related to each other.

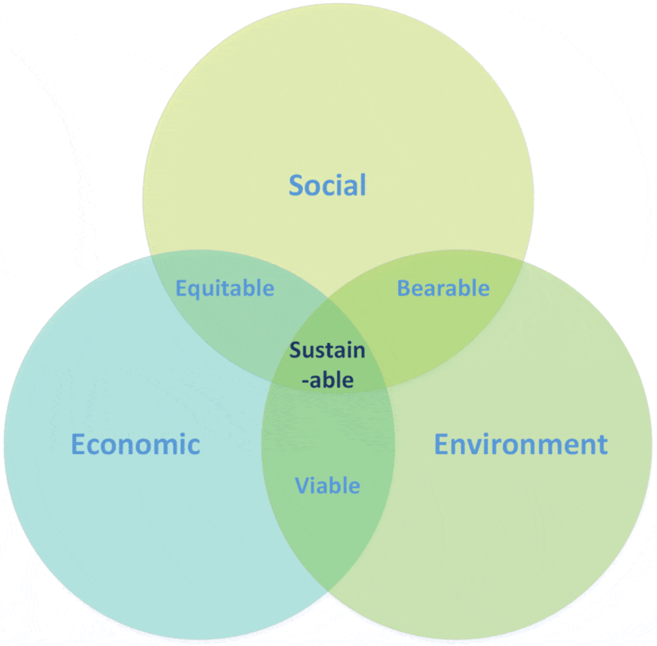

Figure 2. Venn diagram of the three dimensions of sustainability. Source: https://circularecology.com/sustainability-and-sustainable-development.html

The first of the three dimensions of sustainability is the environment (or the environmental dimension of sustainability). To keep the environment healthy it is necessary to avoid degradation of ecosystems. This allows gaining ecosystem services, which refers to a variety of material and social benefits that humanity can use to enhance its own processes (and that can affect many sectors of human activity) [5]. Keeping pollution low, good levels of biodiversity and managing land use and exploitation of the most basic resources such as food, water and energy resources are some of the main approaches to guarantee that the environmental dimension of sustainability is respected.

The second dimension, the social dimension of sustainability, refers to safeguarding certain moral values: peace, security, social justice, reduced poverty, human and labour rights, proper human settlement development and proper relationship of humanity to the natural environment (such as stop considering “nature” as a commodity and favour human education including concepts such as social ecology) are some of the main concepts [6].

Economy is the third dimension of sustainability. Basically, the economic dimension of sustainability revolves around the ideas that economic growth must be decoupled from environmental degradation and that nature must be considered as an economic externality (the aforementioned concept of “ecosystem services” precisely favours that idea) [5]. Different economy model concepts and attitudes regarding market regulation have been designed for the purpose of improving this dimension of sustainability. However, the key point is how to decouple environmental degradation from economic growth, which is an issue addressed by ecological economics and similar scientific frameworks. It has been concluded that although technology efficiency improvements applied to the current production system can reduce resource consumption, it will not make significant changes [7]. Instead, what is required for accomplishing is to reformulate the current linear economy production system. As a result of this need, the concept of circular economy has been formulated and has gained significant popularity [8].

Circular economy is comprised by the basic steps of linear economy (resource extraction, manufacturing and disposal), but additionally it suggests that materials that were to be disposed because they have reached the end of the linear economy lifecycle were instead transformed into a resource to be extracted. Thus, circular economy revolves around the idea of transforming waste into a resource, to form a closed loop of materials. The formation of this loop would allow a reduction of resource extraction and energy consumption, hence reducing significantly the pressure on the biosphere when compared to linear economy [8]. Production systems based on circular economy would achieve “value” not by increasing production, but by keeping the same materials available for longer time within the new lifecycle loop of “make-use-reuse-remake-recycle” [2]. Circular economy could be defined as a restructuring of production systems with the implementation of processes that would allow maximizing athe efficiency in the use of resources (including energy), recycling the highest possible amount of waste and minimizing the emissions. An example for the energy sector is the use of renewable energy.

However, the transition from linear economy to circular economy presents many challenges. The key challenge to enable a transition from linear to circular economy is convincing a significant amount of agents and decision-makers across various sectors of human activity (such as economists, politicians, company leaders or policy makers), but it is also important to convince the general public and carry dissemination efforts to increase a positive public reception of those new concepts of economy models [9]. In Figure 3 the differences between linear economy and circular economy are shown.

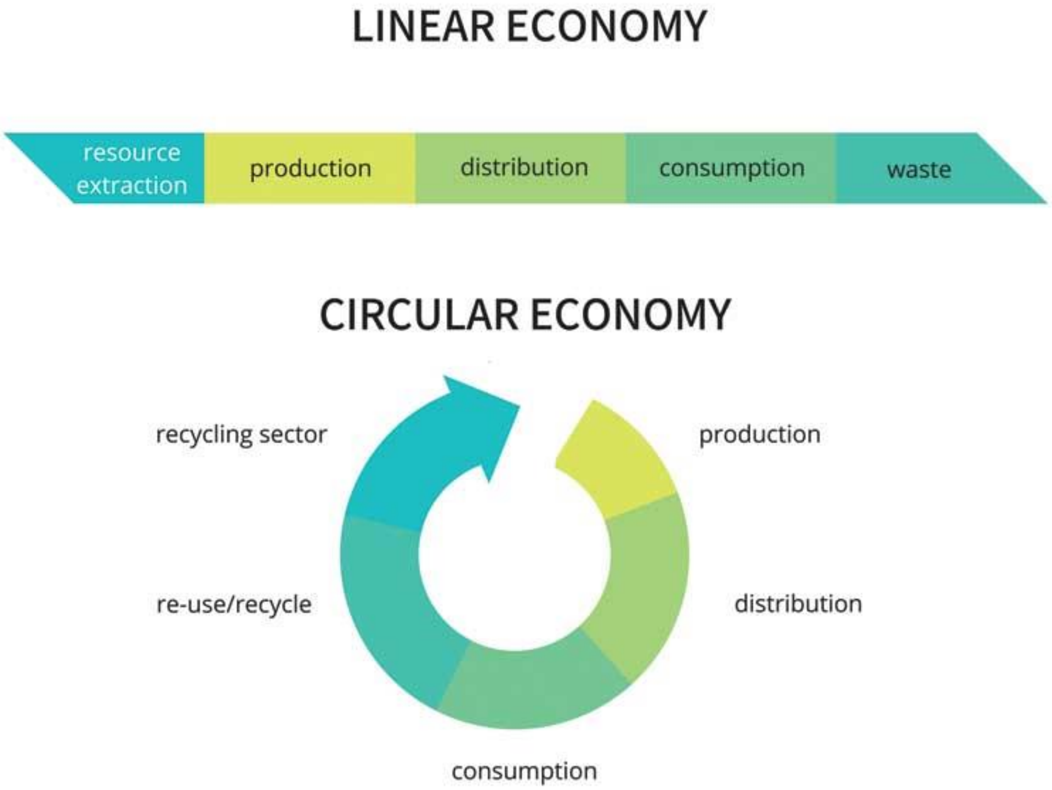

Figure 3. Differences between linear and circular economy. Extracted from https://www.constructionspecifier.com/the-circular-economy/

Most decision-makers who primarily base their decisions on economic criteria see the circular economy concept with scepticism. On the other hand, decision-makers that use not only economic but also social and environmental criteria can tend more favourable to the promotion of circular economy based production systems.

Either way (but especially for the economic criteria based type of decision-maker) to increase awareness of circular economy and its potential benefits it is important to conduct demonstrative projects. Based on the assumption that a city can represent a microcosm of worldwide economy, different municipalities have attempted to reproduce the transition from linear economy to circular economy within their area (known as “circular cities”), both as demonstrative projects and as scientific experiments to gather insight about the key drivers of circular economy transition [8–11]. Some of the conclusions extracted from these experiences are that circular economy implementation requires:

1. Systemic changes through the coordination of public administrations from various sectors and from various levels of governments’ hierarchies
2. The use of intentionally designed business models based on concepts as Product-Service System (PSS) or Re-Distributed Manufacturing (RdM). The “intentionally design” term means that proper business models must be designed ad-hoc for each sector of human activity because it does not exist a universal solution (apart from the generic concepts such as sustainability or circular economy)
3. An upgrade of current policies to favour changes in business models based on circular economy concepts

1.3 The role of the sanitation system in achieving sustainability

The urban water cycle is an essential service of human civilisation (an overview of the urban water cycle is shown in Figure 4). Specifically, it allows potable water supply for both domestic and industrial uses, and it enables the collection, transport and treatment of wastewater (the sanitation system). Overall, the urban water cycle can be assimilated to a circular economy based production system: freshwater resources are exploited to produce potable water, which are consumed through industrial and domestic uses, and wastewater is produced afterwards. Finally, wastewater is collected and treated; so it may be returned clean to the freshwater masses and the production cycle is restarted downstream [12].

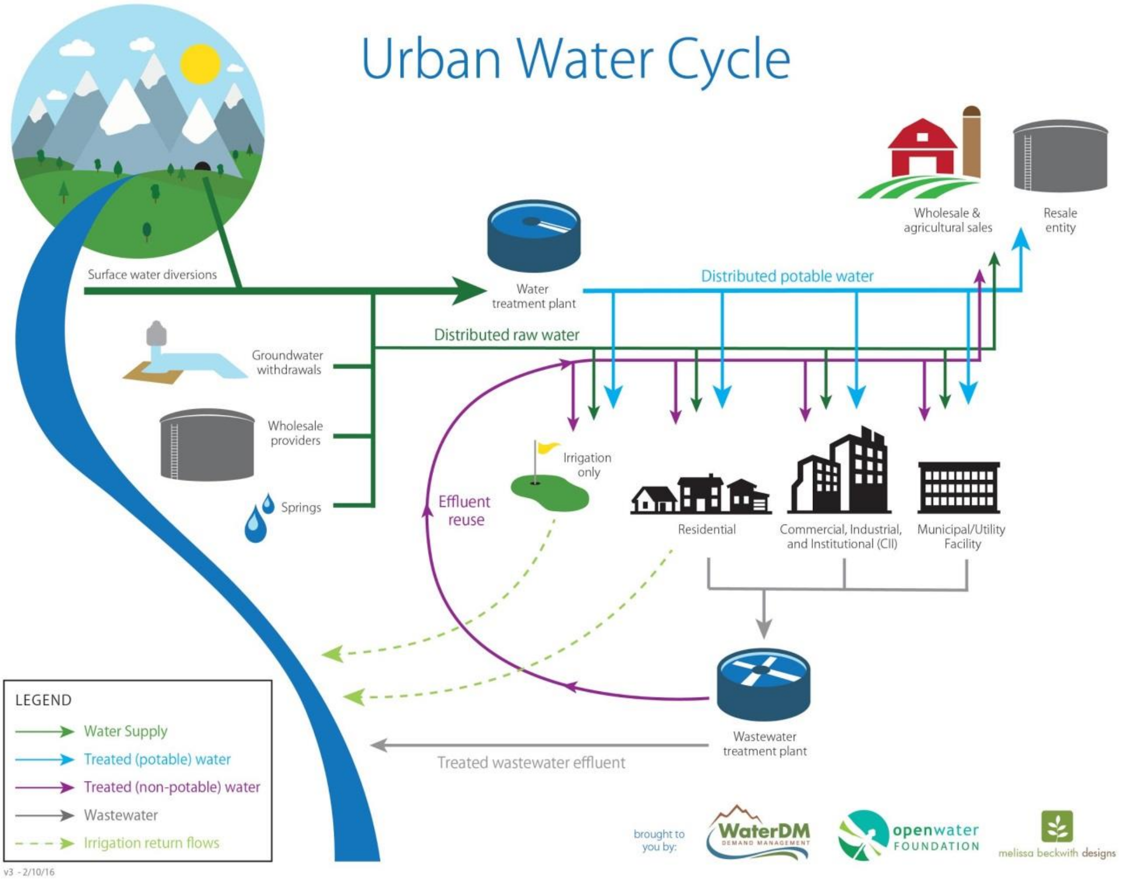

Figure 4. Urban water cycle overview. Extracted from https://www.waterdm.com/publications-reports

Wastewater is composed primarily of water and organic substances that come from human excreta, household, commercial and industrial drains within the collection area and other spills. Once collected through the sewer systems, wastewater reaches the waste water treatment plants (WWTPs). In the WWTPs, wastewater goes through the following processes (that together form the “water line” in WWTPs):

1. Pretreatment: particulate solids such as sand, grit, grease and generic trash (also called screenings) are the first elements separated from wastewater to avoid erosion damage of the particulate material on further pipelines and pumps of the WWTP.
2. Primary treatment: dissolved organic and inorganic matter that can be settled are separated in this process. That way, only dissolved substances unable to be settled by physical separation processes remain in the water flow.
3. Secondary treatment: also called biologic treatment, this process is based on the use of microorganisms to eliminate the remaining dissolved organic substances from wastewater: mostly carbon and nitrogen based molecules, but also phosphorous related molecules, although the latter are usually eliminated by means of chemical precipitation also at this stage (specifically, by addition of ferric chloride or a similar product).

The separated substances along the aforementioned steps 2 and 3 of the water line are the origin of sewage sludge. Most WWTPs have a second treatment line focused on the treatment of the sewage sludge, known as the “sludge line”. The usual processes involved in the treatment of sewage sludge are:

1. Sludge thickening: a concentration of the raw sludge by physical processes (usually gravitation settling, dissolved air floating or centrifuge). This process allows reducing significantly the volume of sewage sludge, facilitating posterior handling.
2. Sludge stabilisation: sewage sludge is formed essentially by organic matter, so it can suffer biological processes such as decomposition, which generates undesired emissions and can be a source of diseases. There are a myriad of processes related to sludge stabilisation with objective of preventing those negative impacts on further steps of sewage sludge handling [13–15]. The most popular is anaerobic digestion, due to its ability to transform a portion of the organic matter into biogas, which is a methane-based gaseous fuel with similar properties to those of fossil fuel gas (also primarily composed by methane). The anaerobic digestion of sewage sludge and all sorts of organic waste is a well-established practice due to its potential to reduce sewage sludge and produce a commodity with potential to generate energy [16,17].
3. Sludge dewatering: this process is aimed at minimize the volume of sewage sludge by extracting the water it contains (usually by centrifuge processes), to provide a solid cake of sewage sludge, much easier to handle than the former liquid fluxes.
4. Sludge disposal: the solid (or semi-solid) cake of sewage sludge is sent from the WWTP to its final disposal site: the conventional disposal way used to be landfilling, but in the

last years land application (as a fertilizer for agricultural purposes) has become a predominant tendency.

5. Return liquors. All the water extracted from steps 1-4 of the sludge line is collected in pipelines separated from those conducting sewage sludge. The liquids collected in these pipelines (which have a high concentration of carbon, nitrogen and phosphorous compounds) are called “return liquors”, and usually they are redirected to the wastewater input at the beginning of the WWTP water line, so they can be treated.

Figure 5 shows a general process diagram of a wastewater treatment plant.

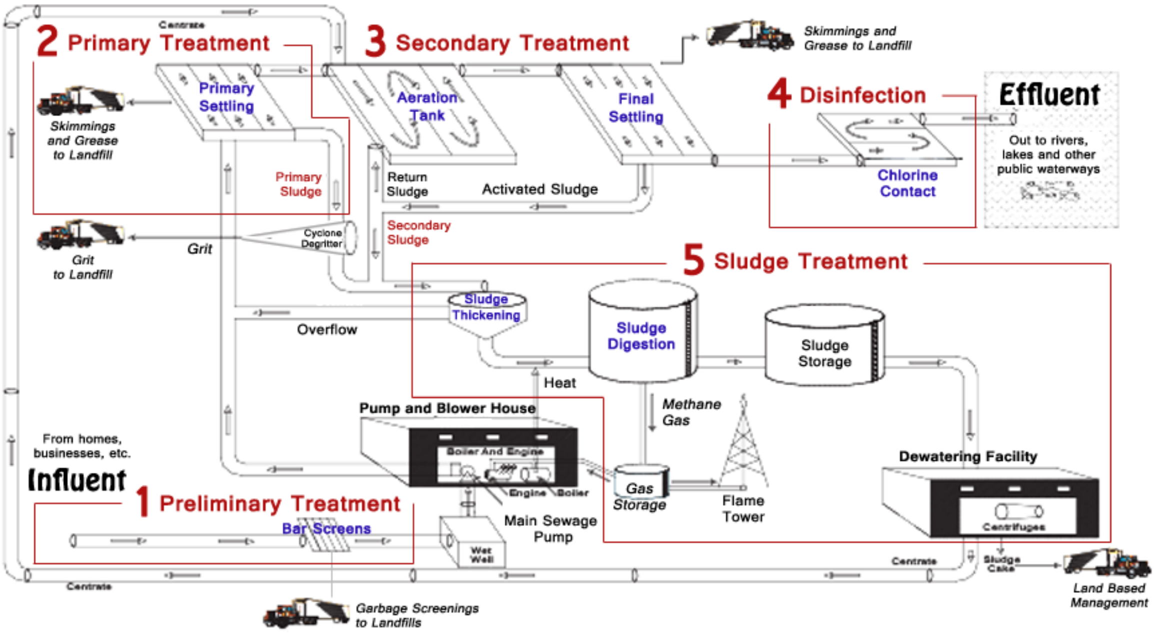

Figure 5. General wastewater treatment plant layout. Extracted from www.mooersproductsinc.com/complete-aeration-systems/

Overall, not only the urban water cycle presents similarities to circular economy (due to the water resource being used and then “recycled” into clean water), but also the sanitation system presents a potential to contribute to sustainability: it enables closing the urban water cycle, while simultaneously producing energy from the sewage sludge and the ultimate fraction of solid waste generated (or biosolid) can be used as an alternative fertilizer. Together with the fact that sanitation is a universal need, these are the main reasons why wastewater treatment is considered a key element in the Water-Energy-Food Nexus (the WEF nexus), which is an essential inter-sectorial leadership strategy aimed at promoting sustainability [18]. Thus, the wastewater sector is essential to achieve sustainability.

1.4 Waste valorisation in the sanitation systems

As already mentioned the transformation of waste into a product or into a useful commodity of the production system is necessary in achieving implementation of circular economy and, thus, a step towards sustainability. This process of closing linear economy into circular economy usually receives the name of waste valorisation. That is, to give "value" to waste. Now, in the context of the global resource crisis and the modern concept of sustainability, the term "value" goes beyond mere economic aspects. However, when related to waste, it usually implies that such material must return to the production system someway as a resource [16].

For the case of the sanitation system, waste valorisation is usually referred to the sewage sludge generated in WWTPs (because water, even as wastewater, is considered as a resource). As such, sewage sludge can generate value through the following strategies:

1. Production of renewable energy carriers: due to its content of organic matter (mostly carbon based compounds), sewage sludge can be used directly as fuel to obtain energy through the oxidation of the organic matter (a process with the generic name of thermal valorisation); alternatively, organic matter can be transformed in energy carriers as biogas and similar gaseous fuels through processes such as anaerobic digestion or gasification [19].
2. Production of organic compounds of high added value: sewage sludge contains a variety of organic molecules that can be extracted through refinery-based processes and these substances can have a significant value in industrial sectors [20].
3. Production of alternative fertilisers: sewage sludge has a significant content of nitrogen, phosphorous and even trace metals within its mixture. Those substances have a high fertilizing potential, so the separation and usage of such components of sewage sludge (such as struvite) present an added value in the agro-food sector [12].

From the previously mentioned general waste valorisation strategies in WWTPs, some processes require a more detailed analysis:

1. Anaerobic digestion: this process enables the transformation of organic matter in biogas, a resource with high circular economy potential (as its considered renewable energy). To properly ensure the operation of the process it is important to consider that it is based on biochemical reactions. Thus, accurate control strategies are required to avoid malfunctions of the process (such as acidification, loss of biomass or microbial inhibition due to excess ammonia or other toxic compounds). Besides, most of the

existent anaerobic digesters are not well optimised (due to e.g. oversizing at the design stage), so there are additional opportunities to increase biogas production by optimising the capacity of anaerobic digestion. To achieve this, external organic wastes are added to digesters, a strategy known as "codigestion". Despite the potential benefits of codigestion, it must be handled with care to avoid undesired malfunctions and keep the performance of the anaerobic digestion process [21].

2. Biogas upgrading: this process aims to purify the biogas into biomethane. This fuel is a substitute of natural gas (a fossil fuel) that can be used without further modifications in the existent gas network, allowing the same performance. Thus, this process enables local production of gas fuel in substitution of a geostrategic resource, such as natural gas that is extracted and transported over thousands of kilometres with expensive infrastructures [22,23].
3. Thermal valorisation: also known as waste-to-energy, it refers to a set of processes that includes incineration. All these processes are based on burning organic matter in industrial furnaces at high temperatures, producing high amounts of energy, ash and fumes. This process also produces a significant amount of emissions and particulate matter that can be a potential pollutant, although different filtering technologies have already been developed and implemented to reduce pollution and even to capture a portion of the emissions produced. Besides, there is an overall negative public perception of the process, not only due to the potential pollution, but also because of the risk of accidents which may occur in this type of plants. However, thermal valorisation allows high reduction of waste volume (transforming it to ashes that can be further refined to extract metals or to be used as fertilizer) and production of energy. Overall, the benefits surpass the potential risks, but a careful planning and risk assessment process is required [24].
4. Land application of sewage sludge cake: there are various ways to dispose of sewage sludge cake. Land application of sewage sludge for agricultural purposes is the main tendency due to its fertiliser ability. Thus, it enables substitution of conventional fertilisers, which rely on phosphate rock mining (another geostrategic resource) and heavy industrial processes. However, sewage sludge land application also presents various risks that must be addressed to ensure the benefits it provides. Crop absorption of metals or other toxic compounds are a risk that is addressed by conducting quality controls of sewage sludge. Runoffs of the applied sewage sludge are another issue with heavy impacts on the local environment, which is attained by the elaboration of fertilisation plans. Also, a minimum degree of hygienization is

required for the sewage sludge to be allowed as fertiliser: each region states a minimum quality threshold based on microbial content indicators according to the Environmental Protection Agency (EPA) biosolids classification [25]; nowadays class B biosolids are still allowed as fertilisers, but policy is going towards more restrictive demands, so an increasing number of regions across the world demands class A biosolids (more restrictive than class B) as the minimum quality to enable land application as disposal pathway for sewage sludge. The degree of sewage sludge hygienization achieved is determined primarily in the sludge stabilisation phase: to achieve class A biosolids it is required that sewage sludge reaches a temperature of at least 55ºC along its treatment process; thus, technologies as thermal hydrolysis or thermophilic anaerobic digestion would serve to this end; however, the first is still a recent development (although it is already being implemented at full scale) and the latter is much less frequent than its counterpart, mesophilic anaerobic digestion process (which only allows achieving class B biosolids because anaerobic digesters operate at around 35-37ºC).

These are significant opportunities for the wastewater sector and different initiatives have been carried to favour the implementation of such strategies: from scientific literature used to gather insight for fundamental science and development of innovative processes [26–28] to international, multidisciplinary projects aimed at identification of potential risks, barriers and developing of guidelines or tools to aid in the transition to circular economy within the sanitation systems [16,29–31].

1.5 The challenge of eco-innovation and implementation of circular economy in WWTPs

Eco-innovation provides a double benefit in order to achieve sustainability because it provides of direct positive externalities to the market by improving the current production system, as well as indirect positive externalities through the reduction in external costs from environmental damage [32]. As there are specific challenges regarding linear to circular economy transition, there are also challenges to properly procure eco-innovation. Actually, circular economy implementation is a type of eco-innovation.

Much discussion has already been done about the process of innovation and eco-innovation, as well as their related barriers [32]. Some of the conclusions of such works indicate that currently the difference between innovation and eco-innovation is not clear because end users still are not able to fully understand the indirect positive externalities of eco-innovation. Since the most common drivers to innovation are demand-side, end-users are the most common stakeholder. Thus, if stakeholders do not account for the added benefits of eco-innovation it will become almost unfeasible; specially for eco-innovation projects that may require high amounts of investment, such as circular economy implementation.

Usually during innovation processes there is a moment where stakeholder confidence on the innovation project is especially low, known as "Valley of Death", until the point that most innovation projects can not get over that point. For the case of eco-innovation projects the Valley of Death is a greater issue than for conventional innovation. Thus, to enable a relative success of eco-innovation projects it is necessary to provide auxiliary tools, such as eco-innovation procurement policies [33].

For the case of circular economy implementation as an eco-innovation process, high amounts of investment are usually required (as any process of business transformation in product systems). Also, due to the changes it may produce, it is important to conduct detailed risk analysis of the correspondent eco-innovation project and consider associated uncertainties to project development as to results expected. Thus, the decision-making process related to circular economy implementation relies on the use of extensive and accurate data.

Considering the multidisciplinary nature of the wastewater sector (because it is a fundamental element of the Water-Energy-Food nexus and thus it generates data from all of its processes), decision-making for implementation of waste valorisation in WWTPs is a significantly complex task. Hence, conventional methods of data collection and processing may consume unachievable amounts of time and resources. And this downside, in the current context of increasingly ever-changing challenges, is a major issue.

When it comes to WWTP planning, there is a considerable amount of unit operations, each with their own possible technologies, and each of those technologies with various possible operation modes (according to parameters such as flow or retention time). The high amount of possible combinations makes a difficult task for conventional decision-makers to properly assess and plan for future WWTP development, while considering new restrictions, policies and opportunities for circular economy implementation. Thus, supporting tools are demanded to enhance such decision-making process.

A number of decision-making and WWTP planning tools has arisen as a result. Some of these tools are focused on modelling a WWTP according to the selected configuration of technologies, as it is the case of the Plant Wide Model (PWM) developed in [34]. Others are focused on enhancing control systems or optimising the operation of determined key processes of the WWTP, as the case of [35], where a tool is designed to enhance the process of biogas upgrading, or in [36], where the objective attained is optimisation of anaerobic digestion. And even some tools have been developed to automatically propose technology configurations of WWTPs, according to a basic description and the desired performance, all by means of artificial intelligence based methods, as shown in [37,38].

However, there is still a lack of accessible tools focused on the last stages of sewage sludge management. There are tools that allow Life Cycle Analysis (LCA), as in [39], but currently the integral assessment of sewage sludge management strategies (including technology assessment in WWTPs, performance estimation and impact and economic analysis of the different sewage sludge disposal pathways) as in issue not fully addressed. One of the reasons is that WWTPs are a functional unit more related to water researchers, while sewage sludge management and valorisation is an issue usually addressed by waste and energy related researchers; besides, to properly characterize many of these steps, a significant amount of data is required, so the relatively limited accessibility of researchers to real case datasets is an important limitation in the development of eco-innovation and circular economy implementation in WWTPs.

The integral environmental, economic and technical analysis from the sewage sludge line to its disposal pathways, while considering potential policies, restrictions and the impacts and potential offsets of both conventional and innovative technologies is a challenge not yet solved. Furthermore, WWTPs can have synergies with other local WWTPs and other waste generators when to evaluate strategies for integral sewage sludge management: examples of such synergies are codigestion and the local centralization of sewage sludge treatment (which as a useful strategy for those processes that couldn't be affordable to implement in each WWTP). For instance, codigestion strategies increase energy feasibility of WWTPs and enable anaerobic digestion as versatile waste receptor sinks [40], although control strategies are highly recommended to guarantee the correct operation of anaerobic digestion [41].

These synergies amongst WWTPs and even external waste producers are opportunities that remain to be comprehensively addressed; an additional level of complexity that is required to tackle in order to provide integral assessments of sewage sludge management in a sanitation system composed of various WWTPs.

This thesis focuses on proposing an approach to integral sewage sludge management for a sanitation system with various WWTPs, while attaining the potential synergies amongst them. Concerns from operators of the case study (that will be described in Chapter 3) involve the need of new tools to polish the decision-making process regarding implementation of waste valorisation processes in WWTPs. It is also important to account for uncertainties to provide an accurate estimation of the impact of the proposals of circular economy implementation.

Since the presented problem is related to decision-making and system analysis, methods related to DSS development are potentially useful [42]. It is proven that features from DSS allow better management in the wastewater sector, especially when confronting uncertainties that might come from different sources [43]. Overall, DSS systems can provide resilience to the management of wastewater systems, hence contributing to increase the overall sustainability.

Also, system analysis and process simulation are useful tools already used to enhance WWTP development planning. So, the use of digital technologies can enable the required intentional design of circular economy processes for each sector, as those methods foster optimisation of material flows and enable careful planning of reverse material flows [9,42]. However, one of the main gaps is related to data collection, integration and analysis. Real case studies - as the one presented in this thesis - integrate a significant amount of data, so they are an opportunity to prove the potential of digital technologies as enhancements of the decision-making process related to implementation of circular economy in WWTPs, while taking care of optimising the integral management of sewage sludge. This thesis has been developed in the framework of an industrial doctorate, working closely with practitioners of the case study, so there is a high availability of data and knowledge from a real sanitation system.

Chapter Two

Objectives

This PhD thesis aims to address the implementation of circular economy in the sanitation system as means to facilitate achieving sustainability. Specifically, develop smart methods to enhance the implementation of waste valorisation processes in WWTPs, with higher ability to address complex problem-solving.

While waste valorisation is a widely known circular economy strategy across sectors, the present work has been focused on developing methods to smooth the most significant bottlenecks of implementation of waste valorisation processes in the sanitation sector (such as information management to assess complex issues). At present, implementation of circular economy in essential services as sanitation and waste management is an emerging concern. This PhD aims to provide ad-hoc, smart, data-driven methods to provide to sanitation practitioners a smooth implementation of waste valorisation processes to achieve a higher degree of circular economy.

This PhD thesis is outlined in different chapters as detailed as follows, according to different objectives related, to achieve the main goal of the improvement of the implementation of waste valorisation processes in WWTPs. Hence, the main objectives of the PhD are:

- To perform a system analysis of the sanitation system's case study, with focus on the WWTPs, the potential waste valorisation processes and identification of specific implementation bottlenecks (Chapter 4).
- To develop methods to smooth the most significant bottlenecks of implementation of waste valorisation processes of the sanitation system and apply to the case study (Chapters 5 and 6). Specifically, simultaneous optimisation of anaerobic digesters of various plants and development of a process simulation-based DSS tool at plant-level are the main methods developed.

Chapter Three

Methodology

3.1 The DSS approach

Conventional decision-making processes lack the required adaptability to overcome present and future challenges, due to their increasing complexity and the lack of improvements on methods of information search and gathering. DSS improve the decision-making process by providing the fittest solutions to complex problems, usually including environmental and economic assessments. That is especially useful for holistic challenges such as sewage sludge management. Examples of the application of DSSs to optimize decision-making regarding WRRFs can be found in recent literature [35,38,44].

To develop new methods to improve the decision-making processes about circular economy implementation in WWTPs, the 5-step process of DSS development in Figure 6 is followed. These are followed as a methodological guideline to sort and process the great amount of available information and also for development of further methods for the sewage sludge valorisation sector.

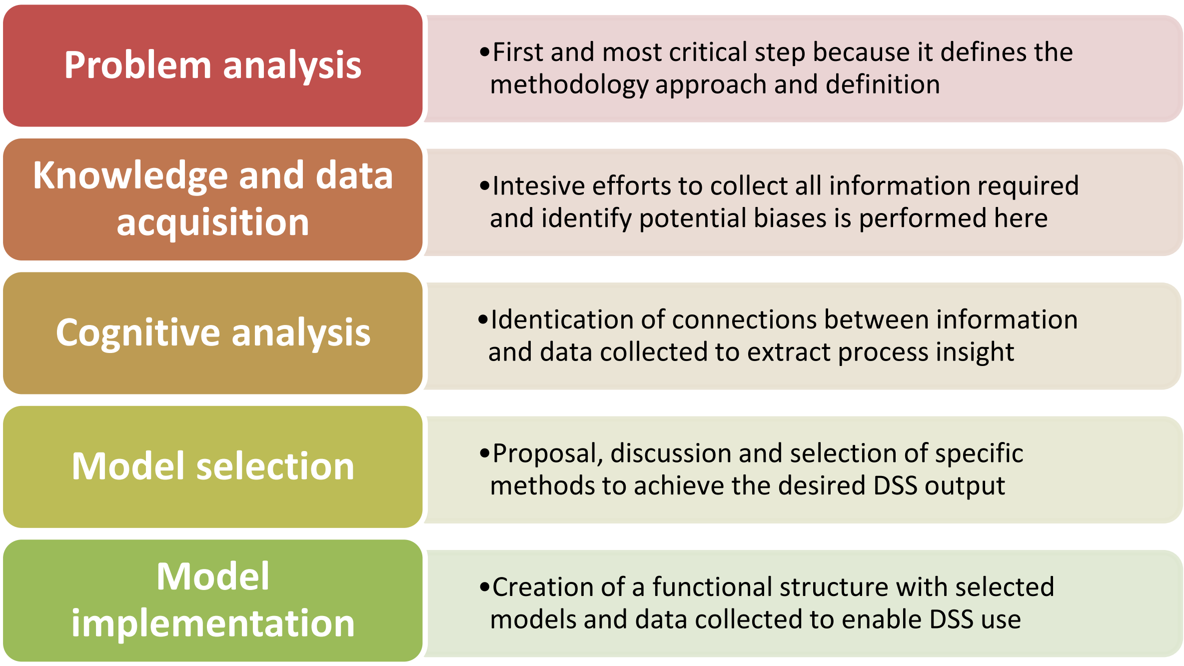

Figure 6. Overview of the 5-step DSS development approach. Adapted from *Decisiones en los sistemas de saneamiento: un poco de ayuda* (Poch,M., Cortés, U., Comas, J., Rodríguez-Roda, I. and Sànchez-Marrè, M.

3.1.1 Problem analysis

As for any methodological framework focused on problem-solving, the first analysis steps are usually the most important because they determine the extent of the solutions provided: the more extensive the framework, the more complex the problem, but also the more holistic the solution. Problem analysis addresses the need to define and study the problem through the following tasks: objective definition; determination of data required for the tool; determination of available data; and determination of procedures required to fulfil the objective.

3.1.1.1 Objective definition

The objective of the methodology is obtaining new tools and proposing strategies to enhance the implementation of waste valorisation related processes in the sector of WWTPs. This is the objective in the thesis framework. To this end, close collaboration with practitioners from the sanitation system of the case study has been performed (in an industrial doctorate framework). Thus, it is required also to state the specific objective of the practitioners and identify the relationships between the case study problem and the thesis problem.

For the case study problem, or the objective of the practitioners of the sanitation system of the case study, the motivation is the enhancement of waste management of sewage sludge in their WWTPs, and thus to obtain assessments and proposals to improve it. That issue has already been mentioned in the introduction section as a background problem (the implementation of waste valorisation processes is bounded by to the usual bottlenecks of implementation of circular economy) that also motivates the ulterior problem that the thesis addresses (the improvement of the decision-making process to enable smoother implementation of waste valorisation processes). Note that such formulation of objectives has been required to differentiate the technical added value of the thesis from the innovation added value (albeit they are highly intertwined).

Overall, the intention of applying the 5-step DSS development is obtaining specific tools to enhance the implementation of sewage sludge valorisation processes. However, before enhancing the implementation process it is required to characterise the current state of implementation of sewage sludge valorisation technologies. That means that the most relevant bottlenecks must be identified, so that the decision-making improvement enables addressing such bottlenecks as best as possible. These bottlenecks, already presented in the introduction section, are as follow:

1. As a circular economy related process, sewage sludge valorisation requires systemic changes through the coordination of public administrations from various sectors and from various levels of governments' hierarchies. That is essentially a bureaucracy and politics related bottleneck which may be hard to directly address through the methodological framework presented (albeit enhancing the decision-making process

might allow practitioners to save time and thus focus more efforts in an efficient communication with other public institutions to achieve these systemic changes).

2. As a circular economy related process, sewage sludge valorisation requires the use of intentionally designed business models based on concepts as PSS or RdM. That is an economic related bottleneck, which can be directly addressed through the presented methodological framework by developing sectorial specific tools such as waste valorisation (there is the "intentional design") focusing on economic assessments.

3. As a circular economy related process, sewage sludge valorisation requires the upgrade of current policies to favour changes in business models based on circular economy concepts. That is an economic and politics related bottleneck that may be addressed through economic assessments but also by scenario comparison: that is, comparing scenarios with different technical restrictions based on potential policy regulations regarding waste valorisation. However, policy uncertainty is a significant issue, that usually it is addressed by assuming higher restrictions over time; in any case, that bottleneck can't be solved directly because of the system of agents that it includes (from regional practitioners of both public and private companies to governments and even international organisations such as the European Commission).

4. As an eco-innovation process relying on significant amounts of investment and on heavy information processing to elaborate proper planning and assessments (due to the complex, multidisciplinary nature of WWTPs as WEF nexuses), implementation of sewage sludge valorisation requires an improvement of the whole decision-making process. Such issue can be directly addressed with the presented methodological framework, since it is designed to develop DSS and, thus, it enables a proper workflow to analyse the problem (implementation of sewage sludge valorisation) and develop solutions.

3.1.1.2 Data required

Data required to accomplish the objective is dependent on the functional unit of the system under study, which is the WWTP. As already mentioned in the introduction section, a WWTP consists of various processes, essentially differentiated by water line and sludge line. Material flows of these lines, as well as energy consumption requirements, are the most basic data required. However, it is also necessary to acquire insight about sewage sludge disposal: which ways are possible (either circular economy related or not), which is their policy context, and estimate both their economic and environmental impact. Also, it is important to gather knowledge about the potential market regarding the commodities that can be produced with sewage sludge valorisation processes (for example the energy, gas and fertiliser markets), and determine quality requirements, economic balances and contributions towards circular economy implementation.

3.1.1.3 Data availability

Data availability is significantly high, since the methodological framework of the thesis has been applied within the organisational structure of the practitioners of the sanitation system under study. Essentially, data sources are as follow:

1. In-line data is usually connected to Programmable Logic Controller (PLC): data included in this format is related to operation and control of WWTPs. It includes wastewater, aeration and sewage sludge pump functioning status, various valves across both water and sludge line (and of biogas), basic analytical probes from the biological reactor and various level probes across water and sludge line. That data is centralized by the PLC, which is used by the practitioner to control the performance of the WWTP. However, current data collected by the PLCs is not available for further external uses.

2. In-line data not connected to PLC and at-line data are both collected and submitted by the operator to a cloud server database: most data regarding characterisation of material flows and energy consumption of the WWTPs can be gathered here for all the WWTPs of the sanitation system (essentially all in-line or at-line measurements). This source of information is by far the most used by practitioners of the WWTP system (alongside with the direct use of PLCs for control and operation purposes).

3. Off-line data is comprised by data regarding punctual analysis and specific reports of the sanitation system can be found in digital format but spread across the cloud server without a proper knowledge management system. Usually feasibility studies, technical project documents and similar documentation that is used just one time by the practitioners can be found in such format.

4. Other knowledge necessary to estimate environmental impacts, economic and policy context insights or estimations of process performance and quality characterisation of material flows can be found across documents, websites, technical guidelines and external scientific literature. Such information is totally external from the case study, albeit potentially necessary to achieve the desired objectives. Additionally, two open-access external databases have been used for benchmarking purposes: the first is the "Wastewater Survey Data" database, from the online tool of the Water Research Foundation (WRF), which contains information about 271 WWTPs from the USA; the second database "Benchmark Database" has been extracted from the ENERWATER H2020 project webpage, and it contains information regarding 252 WWTPs from Europe.

3.1.1.4 Procedures required

Within the 5-step DSS development methodological framework, specific procedures to achieve the objectives are as follows:

1. System analysis: characterise inputs, outputs, bottlenecks, risks and opportunities of both the current WWTPs of the sanitation system and the waste valorisation processes to implement.
2. Elaborate mass and energy balances to determine the potential of circular economy of WWTPs, and estimate the economic and environmental impacts of new waste valorisation processes and strategies on such balances. Acknowledging uncertainty is also necessary to provide confidence intervals.
3. Design strategies that might enable synergies amongst WWTPs and other industries of the region (following the co-digestion opportunity to increase biogas production).
4. Produce scenario simulations to gather insight about the impact on the whole sanitation system of different waste valorisation strategies or potential restrictions.
5. Enable automatic information processing to produce high quality information, considering that the end user of those tools to be developed would be a decision-maker. Key Performance Indexes (KPIs) are a useful technique to provide such holistic assessments to end-users.

3.1.2 Knowledge and data acquisition

A standardised set of measurements has been collected from each WWTP of the sanitation system with the objective of performing a benchmark and classify them according to their performance and technology configuration. Table 1 indicates acquired dataset for each WWTP.

Table 1. Summary of data acquired for the case study

WWTP ambit	Classification of process analysis	Variable name	Units	Frequency of measurement (year^{-1})	Uncertainty of measurement (%)
Water Line quality	At-line	BODin (Inflow Biochemical Oxygen Demand)	mg/l	150	18
		BODout (Biochemical Oxygen Demand)	mg/l	150	
		CODin (Inflow Chemical Oxygen Demand)	mg/l	150	16
		CODout (Outflow Chemical Oxygen Demand)	mg/l	150	
		Nin (Inflow Total Nitrogen)	mg/l	150	15
		Nout (Outflow Total Nitrogen)	mg/l	150	
		Pin (Inflow Total Phosphorous)	mg/l	150	12
		Pout (Outflow Total Phosphorous)	mg/l	150	
		NH4in (Inflow Ammonium)	mg/l	126	12
		TSSin (Inflow Total Suspended Solids)	Kg	128	18
		TSSout (Outflow Total Suspended Solids)	Kg	128	
	In-line	Conductivity	µS/cm	365	?
		pH	ut. pH	365	?
		Biological reactor temperature	ºC	319	?
Sludge Line quality	At-line	Dewatered sludge solids content	%MS	50	5
		Dewatered sludge volatile solids content	%VSS	50	5
		Primary sludge solids content	%MS	100	?
		Primary sludge volatile solids content	%MSV	100	?
		Biological sludge solids content	%MS	149	?
		Biological sludge volatile solids content	%MSV	149	?
Water Line and Sludge Line material flows	In-line	Dewatered sludge production	Kg/d	365	?
		Biogas production	Nm3/d	365	?
		Influent wastewater flow	m3/d	365	5
		Efluent wastewater flow	m3/d	365	5
		Primary sludge flow	m3/d	365	5
		Biological sludge flow	m3/d	365	5
		Ferric chloride solution inflow	Kg/d	365	?
Energy consumption	In-line	Energy consumption	kWh/d	365	?
		Energy production	kWh/d	365	?

On the other hand, an extensive knowledge gathering process has been performed. At least one visit has been carried for all the WWTPs with higher daily treatment capacity than 500 m^3, and their main technology configurations have been identified. Also, meetings with practitioners of the case study have been done to identify and update all issues regarding sewage sludge valorisation. Some local experiences about circular economy implementation projects, closely related to WWTP sewage sludge valorisation, have been recorded through punctual meetings with local actors.

Besides, a state of art of sewage sludge valorisation processes has been performed from both technical documentation and research articles. Such information has been used to increase the accuracy of estimations regarding the impact of implementation of sewage sludge valorisation processes as well as to identify potential bias and state all required assumptions.

3.1.3 Cognitive analysis

Cognitive analysis revolves around maximising the performance of the obtained information and data gathered, usually using data-processing, statistical methods to identify behavioural models to gather knowledge that would be later used for the next steps of the DSS development.

However, to perform a proper cognitive analysis, it is necessary to differentiate between the cognitive analysis of quantitative and qualitative data, both of which are significantly abundant in the case study. Conducting cognitive analysis of qualitative data allows gaining insight towards more accurate model selection and implementation. On the other hand, cognitive analysis of quantitative data is necessary to identify behavioural models of the system's processes under study.

On one hand, regarding cognitive analysis of qualitative data, much has been already mentioned about WWTPs technological layout, and bottlenecks to implementation of sewage sludge valorisation. For instance, the fact that WWTPs consist of the water line and the sludge line, each of those composed of different combinations of technologies increases the complexity of the problem. Even more, the existence of multidisciplinary issues regarding optimal WWTP operation makes highly necessary the use of scenario based assessments. These scenarios are based upon the basics characteristics of the WWTP under study, and an array of performance indicators are estimated for each of them. However, taking into account each technological configuration with all possible environmental, economic and policy constrains at the same time implies a high number of combinations. Besides, the solutions provided, even in the form of assessments, can hardly include all the necessary information in an appropriate format for end-user decision-makers. Thus, optimal WWTP development planning is highly dependent on scenario analysis and integrated assessments.

However, a common trend in sewage sludge valorisation and circular economy implementation in WWTPs is that anaerobic digestion is a crucial process (due to its capacity to reduce sludge production and produce an energy carrier such as biogas). Then, its optimisation provides a high impact: codigestion and centralization of sewage sludge anaerobic digestion are the most common strategies to optimise anaerobic digestion processes.

On the other hand, regarding cognitive analysis of quantitative information, most of the available data is related only to material flows and their basic characterisation. This enables the calculation of mass balances, KPI benchmarking and process simulation of the currently full-scale existent processes. However, further calculation of potential impacts of innovative technologies, as well as economic and environmental impact assessments, are based on estimations. Thus, identification of uncertainties (and of assumptions made) is an essential requirement. Also, it is also important to determine the tolerance of uncertainty for the WWTP sector. WWTPs are dynamic systems highly dependent on their influent, and each WWTP presents a set of well-known daily behaviours. But when it comes to assess (or estimate) the performance of the WWTP within higher periods of time (weeks or months) these behaviours become more distorted due to the inner dynamics of the WWTP system and the properties of its wastewater. Besides, for all the “big picture” performance assessments of WWTPs that are used in most technical projects, many assumptions and estimations are made based on average performance of the WWTP’s processes. As a result, in the WWTP sector a relatively high tolerance of uncertainty has been adopted, as estimated by performing meetings with WWTP’s practitioners and analysing basic mass balance uncertainty propagation: at least, for the most precise, engineering projects estimations, uncertainties around 10-20% are tolerated; while for the gross estimations, related to concept engineering phases, uncertainties around 30% are usually tolerated. In any case, note that these values are used only as reference values of tolerated uncertainty, and for most of the data calculations correspondent uncertainty is calculated.

Finally, limitation of data is a significant issue. Current data available from cloud server database is limited to a single value each day, at the best. Thus, it is not possible to identify daily behavioural models (although general performance of each WWTP can still be estimated from annual datasets). It would be necessary to improve on-line data accessibility managed by PLCs to allow analysis about daily variations. On the other hand, the required knowledge to estimate the performance of sewage sludge valorisation processes and other useful data to elaborate economic, environmental and risk assessments is dispersed through scientific literature or other technical documents. Thus, knowledge management systems are highly encouraged to improve knowledge accessibility.

3.1.4 Model selection

Scenario simulation is a promising technique to address the high amount of combinatorial options regarding WWTP planning (such as technologies, operation parameters and other environmental and economic constraints). Simulation software allows the estimation of a system output in accordance to its properties (which depends on a set of input data and on its configuration). Such technique is convenient to represent the behaviour of real systems. However, to acquire reliable results it is necessary the use of data and knowledge of good quality; otherwise, uncertainties of the simulation may exceed the desired tolerance of uncertainty. Simulation processes in WWTPs include mass and energy balances, as well as integrated economic assessments (if enough data is acquired) and environmental impact estimation. Although simulation of such multidisciplinary processes imply the handling of multiple variables each of them with their own physical meaning in the real system, the use of KPIs are useful as mean of expressing the simulation output in a condensed format.

Such techniques have been applied to improve WWTP planning and implementation of innovative processes [34,45,46], sometimes coupled with elements related to DSSs. Actually, both simulation- and DSS-based procedures have the potential to overcome challenges of sewage sludge valorisation and WWTP proper sustainable planning. Thus, DSS coupled with plant simulation is a promising strategy for providing integrated assessments. Since the current thesis framework is developed within a case study with high data availability, extensive simulation and validation studies can be performed. Thus, it is viable to develop a solution that could fully merge simulation and DSS methods to develop solutions for WWTP planning.

Here, model simulation and DSS have been implemented in a software tool in order to provide insight from the processes under study. Its design is focused on scenario simulation, each composed of the WWTP configuration and a set of input data (mostly characterisation of WWTPs flows). To this end, KPIs are calculated and organized according to a certain importance hierarchy: the objective of the KPIs hierarchy is distributing the information across three levels of decision-making (a first layer of few strategic KPIs, Layer 1, more suited to get quick analysis and a big picture of each scenario; a second layer, Layer 2, with further KPIs focused on the general performance of the WWTP, more suited to daily practitioners of WWTPs, allowing precise performance estimation; and a third layer, Layer 3, with full technical detail of the most significant process variables); overall, this hierarchical organisation of KPIs allows end-users to quickly find those KPIs most relevant to their respective query or decision-making process. The selected method will be identified onwards on the document as SIM-SAD (from the Catalan word *Simulador* and the acronym SAD, the Catalan equivalent for DSS).

3.1.5 Model implementation

Model implementation refers to the creation of functional software capable of running the selected models, modify them according to the input of each case study and obtain proper assessments that would encompass the output of the selected models.

The model presented is implemented via a software tool, aimed at developing a set of toolboxes for of the processes to be simulated and a correspondent tailored process library to encompass them all. The tool is developed in MATLAB-SIMULINK environments: the first provides a computing and programming platform widely used and convenient for prototyping and development of programming frameworks; on the other hand, SIMULINK allows visual programming of the processes involved in the tool, considering each one as a system block (i.e., a self-contained unit of code related to at least one process of the system).

The aim of the DSS-WWTP simulator tool is to provide an assessment for different combinations of existing or potential technologies by simulating each scenario and assessing the performance of the WWTP with the KPIs. Thus, the use of a library for the different implemented technologies and the KPIs as the output of the simulation for assessment is a core feature of the presented tool. Overall, the developed DSS-WWTP simulator has two main modules: the process library and the WWTP simulator.

To implement the model, the following processes are briefly explained and classified as external to the tool (A1-A4) or internal to the tool (B1-B3). First, the processes external to the tool are introduced:

A1. Matlab data import: in this process data is imported into the tool, usually from datasheets available from the central database of the case study. Note that it is important that data source is formatted in a consistent and homogenized way to allow convenient data import and handling.

A2. Data cleaning: in this process outliers in data are removed and interpolation is carried out to fill missing data instances in the time-series.

A3. Creation and assignation of variable tags and adaptation to Simulink format: for each variable used later by the model, a tag is assigned for further reference and standardisation within the code. Variable tags are created manually on a excel spreadsheet, which is imported into Matlab as a string array; that array is then used to replace the default variable tags generated by Matlab data import (step A1). Finally, the time vector (arranged in a daily based timestamp) is adapted to the required target format.

A4. Data export from Matlab to Simulink interface: data input time-series created and formatted along processes A1-A3 are routed to Simulink input data blocks, in Matlab timetable format.

After steps A1-A4, internal tool processes are detailed:

B1. WWTP processes and technology implementation: since the tool is aimed at simulation with specific processes of the sludge line of the WWTPs, in this step the processes are implemented thoroughly. To this end, several steps have been performed as follows:

1. Identification and selection of relevant unit operations, namely: Sewage sludge thickening, sewage sludge pretreatment, anaerobic digestion, sewage sludge dewatering, sewage sludge drying, sludge thermal valorisation and biogas valorisation.
2. For each unit operation, identification and selection of the most relevant technologies that can full the correspondent process.
3. Identification of input and output flows for each unit operation, as well as data required to properly characterize each one.
4. Identification of data availability from the case study to allow implementation and simulation of each process. That is, determine whether data is available in the case study databases or whether if it can be estimated using available information.

The implemented processes resulting from this B1 stage are shown in Table 2, which shows the complete library of simulation blocks implemented.

Table 2. Simulation blocks implemented in the SIM-SAD tool (B1 stage). Input and output variables, as well as the correspondent data source and calculation, are shown below, classified according to the unit operation of the sludge line of the WWTP they correspond.

SEWAGE SLUDGE LINE	Input variables	Input variables data source	Output variables	Output variables calculation
A. Sewage sludge thickening				
1. Default (primary and biological sludge blending)	Q_{ps}: primary sludge flow (m3/d)	Data measurement	Q_{ts}: thickened sludge flow (m3/d)	$Q_{ts} = Q_{ps} + Q_{bs}$
	Q_{bs}: biological sludge flow (m3/d)		S_{ts}: thickened sludge solids (%)	$S_{ts} = \left(\frac{S_{ps}}{Q_{ps}} + \frac{S_{bs}}{Q_{bs}}\right) \cdot Q_{ts}$
	S_{ps}: primary sludge solids (%)		VS_{ts}: thickened sludge volatile solids (% over total solids)	$VS_{ts} = \left(\frac{VS_{ps}}{Q_{ps}} + \frac{VS_{bs}}{Q_{bs}}\right) \cdot Q_{ts}$
	S_{bs}: biological sludge solids (%)			
	VS_{ps}: primary sludge volatile solids (% over total solids)			
	VS_{bs}: biological sludge volatile solids (% over total solids)			

Table 2 (continuation, block B)

SEWAGE SLUDGE LINE	Input variables	Input variables data source	Output variables	Output variables calculation
B. Sewage sludge pretreatment (before anaerobic digestion)				
1. Default (no pretreatment)	Q_{ts}: thickened sludge flow (m3/d)	Simulation block A	Q_{pts}: pretreated thickened sludge flow (m3/d)	$Q_{pts} = Q_{ts}$
	S_{ts}: thickened sludge solids (%)		S_{pts}: pretreated thickened sludge solids (%)	$S_{pts} = S_{ts}$
	VS_{ts}: thickened sludge volatile solids (% over total solids)		VS_{pts}: pretreated thickened sludge volatile solids (% over total solids)	$VS_{pts} = VS_{ts}$
	T_{ts}: thickened sludge temperature (ºC)	Data measurement	BMP_{Raw}: biomethane potential (biogas Nm3/tonne of volatile solids) – as a function of hydraulic retention time (HRT)	$BMP_{Raw}(HRT) = 918 \cdot \frac{HRT}{HRT + 40}$
			T_{pts}: pretreated thickened sludge temperature (ºC)	$T_{pts} = T_{ts}$
2. Thermal hydrolysis				
2.1. Sludge dewatering before thermal hydrolysis	Q_{ts}: thickened sludge flow (m3/d)	Simulation block A	Q_{tphs}: thickened pre-hydrolysis sludge flow (m3/d)	$Q_{tphs} = Q_{ts} \cdot \frac{S_{ts}}{S_{tphs}} \cdot 0{,}9$
	S_{ts}: thickened sludge solids (%)		S_{tphs}: thickened pre-hydrolysis sludge solids (%)	$S_{tphs} = 16{,}5\ \%$
	VS_{ts}: thickened sludge volatile solids (% over total solids)		VS_{tphs}: thickened pre-hydrolysis sludge volatile solids (% over total solids)	$VS_{tphs} = VS_{ts}$
			$K_{polipht}$: dewatering polyelectrolyte consumption (kg/d)	$K_{polipht} = 10 \cdot Q_{ts} \cdot S_{ts}$
			E_{pht}: energy consumption (kWh/d)	$E_{pht} = 1{,}33 \cdot Q_{ts}$

Table 2 (continuation, block B – 2.2)

SEWAGE SLUDGE LINE	Input variables	Input variables data source	Output variables	Output variables calculation
2.2. Thermal hydrolysis core	Q_{tphs}: thickened pre-hydrolysis sludge flow (m3/d)	Simulation block B – 2.1	Q_{ths}: hydrolysed sludge flow (m3/d)	$Q_{ths} = Q_{tphs} \cdot \frac{S_{tphs}}{S_{ths}}$
	S_{tphs}: thickened pre-hydrolysis sludge solids (%)		S_{ths}: hydrolysed sludge solids (%)	$S_{ths} = 10\%$
	VS_{tphs}: thickened pre-hydrolysis sludge volatile solids (% over total solids)		VS_{ths}: hydrolysed sludge volatile solids (% over total solids)	$VS_{ths} = VS_{tphs}$
			Q_{TH}: thermal hydrolysis heat demand (kWh/d)	$Q_{TH} = 31{,}7 \cdot Q_{tphs}$
			BMP_{TH}: biomethane potential (biogas Nm3/tonne of volatile solids) – as a function of hydraulic retention time (HRT)	$BMP_{TH}(HRT) = 918 \cdot \frac{HRT}{HRT + 24}$
			T_{ths}: hydrolysed sludge temperature (ºC)	$T_{ths} = 37$

Table 2 (continuation, block C)

SEWAGE SLUDGE LINE	Input variables	Input variables data source	Output variables	Output variables calculation
C. Anaerobic digestion				
1. Default (single stage mesophilic digestion)	Q_{din}: anaerobic digestion inflow (m3/d)	Simulation block B – 1 (if default process selected) OR Simulation block B – 2 (if thermal hydrolysis process selected)	Q_{dout}: anaerobic digestion outflow (m3/d)	$Q_{dout} = Q_{din} \cdot 65\%$
	S_{din}: anaerobic digestion inflow solids (%)		S_{dout}: anaerobic digestion outflow solids (%)	$S_{dout} = S_{din} \cdot 65\%$
	VS_{din}: anaerobic digestion inflow volatile solids (% over total solids)		VS_{dout}: anaerobic digestion outflow volatile solids (% over total solids)	$VS_{dout} = VS_{din} \cdot 80\%$
	$BMP(HRT)$: biomethane potential (biogas Nm3/tonne of volatile solids)		Q_{bt}: total biogas produced	$Q_{bt} = Q_{din} \cdot S_{din} \cdot VS_{din} \cdot \cdot BMP(HRT_{AD})$
	T_{din}: anaerobic digestion inflow temperature		Q_{AD}: anaerobic digestion heat demand	$Q_{AD} = V_{AD} \cdot 0{,}39 + Q_{din} \cdot \cdot (37 - T_{din}) \cdot 1{,}17$
	V_{AD}: anaerobic digestion volume (m3)	Parameter set at 10000 m3 (adapted to each case study)	COD_{kdin}: anaerobic digester inflow chemical oxygen demand (kg)	$COD_{din} = Q_{din} \cdot S_{din} \cdot VS_{din} \cdot 1{,}42$
	HRT_{AD}: anaerobic digestion hydraulic retention time (d)	Parameter set at 25 days (adapted to each case study)	COD_{kdout}: anaerobic digester outflow chemical oxygen demand (kg)	$COD_{dout} = Q_{dout} \cdot S_{dout} \cdot VS_{dout} \cdot 1{,}42$
			EM_{btg}: emissions from biogas leakages (kg CO2/d)	$EM_{btg} = Q_{bt} \cdot 5\% \cdot 1000 \cdot \frac{1}{293 \cdot 0{,}082} \cdot \cdot (CH4_{bt} \cdot 16 \cdot 25/1000 + (1 - CH4_{bt}) \cdot 44/1000)$

Table 2 (continuation, block D and block E)

SEWAGE SLUDGE LINE	Input variables	Input variables data source	Output variables	Output variables calculation
D. Sewage sludge dewatering				
1. Default (centrifuge dewatering)	Q_{cin}: dewatering inflow (m3/d)	Simulation block C – 1	K_{fd}: mass of dewatered sludge (kg/d)	$K_{fd} = Q_{cin} \cdot 10^3 \cdot \frac{S_{cout}}{S_{cin}} \cdot 0{,}9$
	S_{cin}: dewatering inflow solids (%)	Simulation block C – 1	S_{cout}: dewatered sludge solids (%)	$S_{cout} = 20\%$
	VS_{cin}: dewatering inflow volatile solids (% over total solids)	Simulation block C – 1	VS_{cout}: dewatered sludge volatile solids (% over total solids)	$VS_{cin} = VS_{cout}$
			K_{polic}: dewatering polyelectrolyte consumption (kg/d)	$K_{polipht} = 10 \cdot Q_{cin} \cdot S_{cin}$
			E_c: energy consumption (kWh/d)	$E_{pht} = 1{,}33 \cdot Q_{ts}$
E. Sewage sludge drying (after dewatering, optional)				
1. Conventional sludge drying	K_{fd}: mass of dewatered sludge (kg/d)	Simulation block D – 1	K_{fs}: mass of dried sludge (kg/d)	$K_{fs} = K_{fd} \cdot \frac{S_{fs}}{S_{cout}}$
	S_{cout}: dewatered sludge solids (%)	Simulation block D – 1	S_{fs}: dried sludge solids (%)	$S_{fs} = 85\%$
	$LHV_f(\%solids)$: lower heating value of sludge as a function of solids content	Punctual laboratory measurement and calibration $LHV_f(\%solids) = 3210 \cdot \%solids - 611{,}3$	LHV_{fs}: lower heating value of dried sludge (kcal/kg)	$LHV_{fs} = 3210 \cdot S_{fs} - 611{,}3$
			EM_{sd}: emissions of sludge drying (kgCO2/d)	$EM_{sd} = 0$ (*air drying agent in a closed loop)
			Q_{sd}: heat demand of sludge drying (kWh/d)	$Q_{sd} = \left(K_{fd} - K_{fs}\right) \cdot 1{,}25$

Table 2 (continuation, block F and block G)

SEWAGE SLUDGE LINE	Input variables	Input variables data source	Output variables	Output variables calculation
F. Sludge thermal valorisation (after drying, optional)				
1. Conventional thermal valorisation	K_{fs}: mass of dried sludge (kg/d)	Simulation block E – 1	K_{ash}: mass of ash (kg/d)	$K_{ash} = K_{fs} \cdot S_{fs} \cdot ASH_{fd}$
	S_{fs}: dried sludge solids (%)	Simulation block E – 1	Q_{comb}: heat from sludge thermal valorisation (kWh/d)	$Q_{comb} = K_{fs} \cdot LHV_{fs}/860$
	LHV_{fs}: lower heating value of dried sludge (kcal/kg)	Simulation block E – 1	EM_{comb}: emissions from sludge thermal valorisation (kg CO2/d)	$EM_{comb} = 0{,}83 \cdot K_{fs}$
	ASH_{fd}: ash content of dewatered sludge (% over total solids)	Punctual laboratory measurement		
G. BIOGAS LINE				
1. Default (biogas cogeneration)	Q_{bt}: total biogas produced (Nm3/d)	Simulation block C – 1	E_{be}: electricity from biogas cogeneration (kWh/d)	$E_{be} = Q_{bt} \cdot CH4_{bt} \cdot 10{,}73 \cdot 35\%$
	$CH4_{bt}$: biogas methane content (% v:v)	Punctual laboratory measurement	Q_{be}: heat from biogas cogeneration (kWh/d)	$Q_{be} = Q_{bt} \cdot CH4_{bt} \cdot 10{,}73 \cdot 40\%$
2. Biogas upgrading	Q_{bt}: total biogas produced (Nm3/d)	Simulation block C – 1	Q_{rng}: biomethane flow (Nm3)	$Q_{rng} = Q_{bt} \cdot CH4_{bt}$
	$CH4_{bt}$: biogas methane content (% v:v)	Punctual laboratory measurement		$EM_{be} = Q_{bt} \cdot 1000 \cdot \frac{1}{293 \cdot 0{,}082} \cdot \cdot \left[\begin{matrix} 95\% \cdot \frac{44}{1000} + \\ +5\% \cdot \left(\begin{matrix} CH4_{bt} \cdot 16 \cdot \frac{25}{1000} + \\ +(1 - CH4_{bt}) \cdot 44/1000 \end{matrix} \right) \end{matrix} \right]$

B2. KPI calculation: within Matlab interface, and using Simulink data outputs from the simulation blocks, KPI calculation is performed. Calculations of each KPI, classification within Layer 1, 2 or 3 (already introduced in section 3.1.4. Model selection), and correspondent data used are shown in Table 3.

B3. KPI data output processing: data from step B2 is sorted (in the previously mentioned Layer 1, Layer 2 and Layer 3 of the hierarchy of KPIs) and is graphically represented. Finally, both KPI time-series data and their correspondent graphs are exported to a excel spreadsheet.

The implementation of the aforementioned steps has allowed creating a Simulink interface; Figure 7 shows a screenshot of the prototype used to implement the SIM-SAD tool.

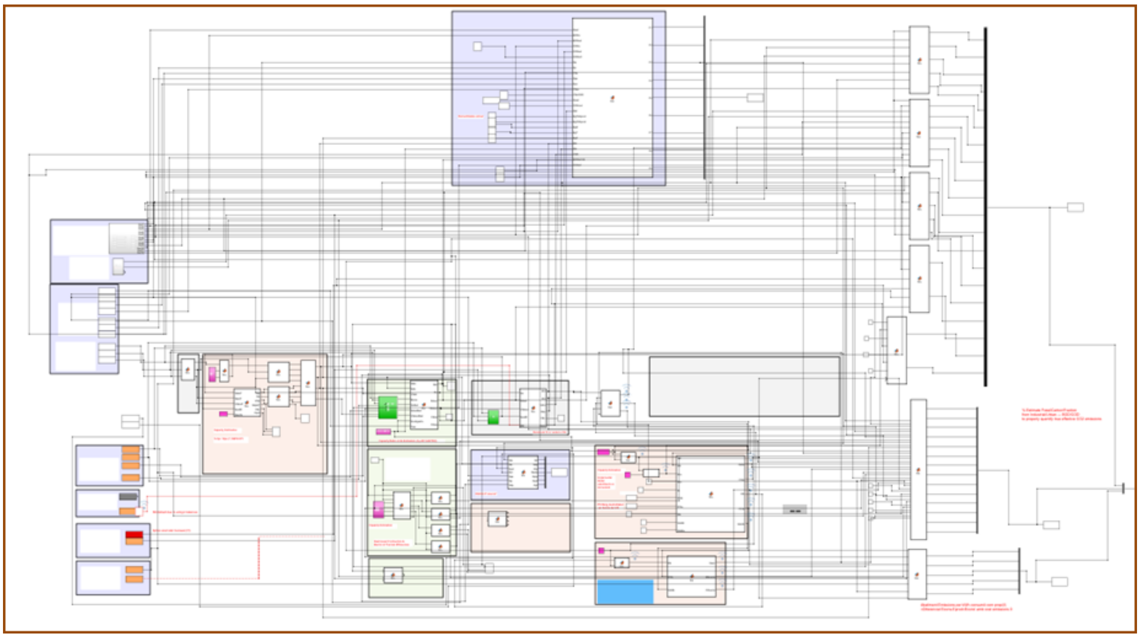

Figure 7. General screenshot of the prototype of the Matlab-Simulink model used to developed the SIM-SAD tool.

Table 3. KPI description, units, calculations and variables used. Sorted by Layer 1 (L1), Layer 2 (L2) or Layer 3 (L3).

KPI	Description	Units	Calculation	Variables
Layer 1 (regional level)				
L1_1	Viability index	-	$\mathit{Not\ implemented}$	
L1_2	Material circularity index	% of maximum recoverable	$\mathit{Not\ implemented}$	
L1_3	Energy self-sufficiency index	% of total consumption	$\frac{Q_{bc}+Q_{be}+Q_{comb}+E_{be}+Q_{rng}\cdot 10{,}73\ kW/m^3{}_{rng}}{E_{cons}+Q_{TH}+Q_{AD}+Q_{SD}}\cdot 100$	Q_{bc}: heat from biogas boiler (kWh/d) Q_{be}: heat from biogas cogeneration (kWh/d) Q_{comb}: heat from sludge thermal valorisation (kWh/d) E_{be}: electricity from biogas cogeneration (kWh/d) Q_{rng}: biomethane flow (kWh/d) E_{cons}: electricity consumed (kWh/d) Q_{TH}: thermal hydrolysis heat demand (kWh/d) Q_{AD}: anaerobic digestion heat demand (kWh/d) Q_{SD}: sludge drying heat demand (kWh/d)
L1_4	Risk & impacts index	% of KPIs over alert threshold	$\mathit{Not\ implemented}$	
L1_5	Economic assessment	NPV (M€)	$\sum_{t=1}^{n}\frac{C_t}{(1+D)^n}-I_0$	n: timespan (y) t: starting period of time (y) C_t: annual cash flow (€) D: discount rate (%) I_0: inversion cost (€)

Table 3 (continuation, Layer 2)

KPI	Description	Units	Calculation	Variables
Layer 2 (plant level)				
L2_1	Organic load	PE*/m3	$\frac{PE}{Q_{in}}$	PE: population equivalent (inhabitants) Q_{in}: wastewater inflow (m3/d)
L2_2	Organic matter elimination	% COD	$\frac{COD_{in} - COD_{out}}{COD_{in}} \cdot 100$	COD_{in}: chemical oxygen demand inflow to WWTP (mg/L) COD_{out}: chemical oxygen demand outflow from WWTP (mg/L)
L2_3	Nitrogen elimination	% total nitrogen	$\frac{N_{in} - N_{out}}{N_{in}} \cdot 100$	N_{in}: inflow total nitrogen (mg/L) N_{out}: outflow total nitrogen (mg/L)
L2_4	Total wastes produced	kg/d	$K_{fd} + K_{fs} + K_{ash}$	K_{fd}: mass of dewatered sludge (kg/d) K_{fs}: mass of dried sludge (kg/d) K_{ash}: mass of ash (kg/d)
L2_5	Total biogas produced	Nm3/d	Q_{bt}	Q_{bt}: total biogas produced (Nm3/d)
L2_6	Anaerobic digester efficiency	% COD converted	$\frac{Q_{bt} \cdot COD_{din}}{0{,}647 \frac{Nm^3}{kg} COD\ max\ biogas\ efficiency} \cdot 100$	Q_{bt}: total biogas produced (Nm3/d) COD_{din}: anaerobic digester inflow chemical oxygen demand (mg/L)
L2_7	Total emissions produced	kg CO2 eq/d	$EM_{rb} + EM_{btg} + EM_{bc} + EM_{be} + EM_{bt} + EM_{st} + EM_{comb}$	EM_{rb}: emissions from biological reactor (kg CO2/d) EM_{btg}: emissions from biogas leakages (kg CO2/d) EM_{bc}: emissions from biogas boiler (kg CO2/d) EM_{be}: emissions from biogas cogeneration (kg CO2/d) EM_{bt}: emissions from biogas torch (kg CO2/d) EM_{sd}: emissions from sludge drying (kg CO2/d) EM_{comb}: emissions from sludge thermal valorisation (kg CO2/d)

Table 3 (continuation, Layer 2)

KPI	Description	Units	Calculation	Variables
L2_8	Energy efficiency (to total flow)	kWh/m3	$\frac{E_{cons}}{Q_{in}}$	E_{cons}: electricity consumed (kWh/d) Q_{in}: wastewater inflow (m3/d)
L2_9	Electricity self-sufficiency	%	$\frac{E_{cons}}{E_{be}}$	E_{cons}: electricity consumed (kWh/d) E_{be}: electricity from biogas cogeneration (kWh/d)
L2_10	Thermal balance	Thermal kW/d	$Q_{bc} + Q_{be} + Q_{comb} + Q_{TH} + Q_{AD} + Q_{SD}$	Q_{bc}: heat from biogas boiler (kWh/d) Q_{be}: heat from biogas cogeneration (kWh/d) Q_{comb}: heat from sludge thermal valorisation (kWh/d) Q_{TH}: thermal hydrolysis heat demand (kWh/d) Q_{AD}: anaerobic digestion heat demand (kWh/d) Q_{SD}: sludge drying heat demand (kWh/d)
L2_11	Energy circularity index	% of maximum recoverable	$\frac{Q_{bc} + Q_{be} + Q_{comb} + E_{be} + Q_{rng}}{PE \cdot 0{,}48\ kW\ potential\ energy/PE}$	Q_{bc}: heat from biogas boiler(kWh/d) Q_{be}: heat from biogas cogeneration (kWh/d) Q_{comb}: heat from sludge thermal valorisation (kWh/d) E_{be}: electricity from biogas cogeneration (kWh/d) Q_{rng}: biomethane flow (m3/d) PE: population equivalent (inhabitants)
L2_12	Waste management cost	€/day	$K_{fd} \cdot \frac{20€}{t} + K_{fs} \cdot \frac{30€}{t} + K_{ash} \cdot \frac{80€}{t}$	K_{fd}: mass of dewatered sludge (kg/d) K_{fs}: mass of dried sludge (kg/d) K_{ash}: mass of ash (kg/d) *Management costs given to each waste can be adapted to each case study
L2_13	OPEX (operational expenditures)	€/day	*Not implemented*	
L2_14	CAPEX (capital expenditures)	€	*Not implemented*	

Table 3 (continuation, Layer 3)

KPI	Description	Units	Calculation	Variables
Layer 3 (process level)				
L3_1	Wastewater flow	m3/d	Q_{in}	Q_{in}: wastewater inflow (m3/d)
L3_2	Biodegradable organic load	%BOD/COD	$\frac{COD_{in}}{BOD_{in}} \cdot 100$	COD_{in}: chemical oxygen demand inflow to WWTP (mg/L) BOD_{in}: chemical oxygen demand inflow to WWTP (mg/L)
L3_3	Phosphorous elimination	% total phosphorous	$\frac{P_{in} - P_{out}}{P_{in}} \cdot 100$	P_{in}: inflow total phosphorous (mg/L) P_{out}: outflow total phosphorous (mg/L)
L3_4	Solids elimination	% solids content	$\frac{S_{in} - S_{out}}{S_{in}} \cdot 100$	S_{in}: inflow total solids (%) S_{out}: outflow total solids (%)
L3_5	Overflow of untreated wastewater	% of flow	$\frac{Q_{in} - Q_{out}}{Q_{in}} \cdot 100$	Q_{in}: wastewater inflow (m3/d) Q_{out}: wastewater outflow (m3/d)
L3_6	Sludge production	kg/m3	$\frac{K_{fd}}{Q_{in}}$	K_{fd}: mass of dewatered sludge (kg/d) Q_{in}: wastewater inflow (m3/d)
L3_7	Sand production	kg/m3	$Not\ implemented$	
L3_8	Grease production	kg/m3	$Not\ implemented$	
L3_9	Screenings production	kg/m3	$Not\ implemented$	
L3_10	Biogas production	Nm3/PE*·year	$\frac{Q_{bt}}{PE \cdot 365}$	Q_{bt}: total biogas produced (Nm3/d) PE: population equivalent (inhabitants)
L3_11	Organic matter balance of anaerobic digestion	%COD input to digesters	$\frac{COD_{kdin} - COD_{kdout} - Q_{bt} \cdot 1{,}545\ kg\ COD/Nm^3{}_{biogas}}{COD_{kdin}}$	Q_{din}: anaerobic digester inflow (m3/d) COD_{kdin}: anaerobic digester inflow chemical oxygen demand (kg) COD_{kdout}: anaerobic digester outflow chemical oxygen demand (kg) Q_{bt}: total biogas produced (Nm3/d)
L3_12	Electricity consumption	kWh/d	E_{cons}	E_{cons}: electricity consumed

Table 3 (continuation, Layer 3)

KPI	Description	Units	Calculation	Variables
L3_13	Energy efficiency (to organic matter)	kWh/kg BOD eliminated	$\frac{E_{cons}}{(BOD_{in} - BOD_{out}) \cdot Q_{in}/1000}$	E_{cons}: electricity consumed (kWh/d) BOD_{in}: inflow biochemical oxygen demand (mg/L) BOD_{out}: outflow biochemical oxygen demand (mg/L) Q_{in}: wastewater inflow (m3/d)
L3_14	Energy efficiency (to total nitrogen)	kWh/kg N eliminated	$\frac{E_{cons}}{(N_{in} - N_{out}) \cdot Q_{in}/1000}$	E_{cons}: electricity consumed (kWh/d) N_{in}: inflow total nitrogen (mg/L) N_{out}: outflow total nitrogen (mg/L) Q_{in}: wastewater inflow (m3/d)
L3_15	Electricity production	kWh/d	E_{be}	E_{be}: electricity from biogas cogeneration (kWh/d)
L3_16	Electricity production efficiency	kWh/Nm3 biogas	$\frac{E_{be}}{Q_{bt}}$	E_{be}: electricity from biogas cogeneration (kWh/d) Q_{bt}: total biogas produced (Nm3/d)
L3_17	Phosphorous elimination efficiency	kg eliminated P/kg ferric salts	$Not\ implemented$	
L3_18	Sludge dehydration efficiency	kg polyelectrolyte/t MS sludge	$Not\ implemented$	
L3_19	Reagent consumption cost	€/d	$Not\ implemented$	

3.2. Optimisation of WWTP co-digestion process

Mathematical optimisation involves the selection of one alternative amongst a set, according to some criterion (that is, the optimisation problem). An optimisation problem can be basically defined as a function $f(x)$, containing an n-variable vector x, where the variable x must be subjected to a process of optimisation, and where additional constraints $g(x)$ may be considered in the optimisation process. The function $f(x)$, also called objective or cost function, encompasses all the possible solutions to the problem (x). The constraints $g(x)$, if applicable to the corresponding optimisation problem, specifies which solutions of the objective function $f(x)$ are feasible. Usually the optimisation problem involves minimisation of the objective function $f(x)$, so the mathematical procedure is aimed at minimising $f(x)$ over the n-variable vector x which conforms the range of available solutions.

Ant Colony Optimisation (ACO) is an algorithm aimed at finding the optimal solution of the optimisation problem posed, -i.e. minimize the objective function $f(x)$ subject to the set of constraints $g(x)$ which apply- which consists in the selection of the best substrates and volumes according to a set of restrictions related to the operation of the anaerobic digester. Besides, the cost function allows quantifying the value of each alternative of the set under optimisation, and has a mathematical expression that varies for each case, but it always involves the calculation of a value or "cost" associated to each alternative according to a set of variables that one way or other are related to the imposed restrictions or other criterion that drives the optimisation procedure.

Due to the high relevance of anaerobic digestion on its own as crucial process for sewage sludge valorisation, a method is developed here in order to optimise anaerobic digestion process. The method selected is based on previous works of optimisation of anaerobic digestion [47], where optimisation of the feed to a single anaerobic digester was performed by means of the ACO algorithm. This algorithm is based on the concepts of the Traveling Salesman Problem (TSP) and the Knapsack Problem (KP), adapted to an evolutionary algorithm.

The Travelling Salesman Problem (TSP) [48] is referred to the optimisation problem posed by the need to optimize (specifically, minimize) the distance that a traveller must do to reach a set of locations; such problem can be expressed as a distance minimisation, restricted by the geographical position of each location of the set, which constitutes the problem definition. On the other hand, the Knapsack Problem (KP) [48] is a traditional combinatorial optimisation problem, where a knapsack with limited weight must be filled with a set of items with a given weight and value each; however, since the knapsack has a weight restriction, the optimisation lies at filling the knapsack with a subset of items so that the accumulated value of the knapsack would be the highest possible.

The resulting behaviour of applying ACO-based methods to the optimisation problem of anaerobic co-digestion is similar to that of ants: it is optimised both the cost of the route and the amount of substrate transported in each route towards the digester. Optimisation algorithms as the ACO allow solving optimisation problems, which are defined by a cost function. The ACO algorithm has been used to minimise a cost function that includes quality and quantity data related to blend composition of anaerobic digestion, while maximising the capacity of biogas produced, as shown in equation 1. It has been applied previously in the work of Verdaguer et al [47] for a similar problem, where it was used to optimise the management of multiple wastewater streams.

$$B = 1/\left\{\sum_{w=1}^{N}\sum_{s=0}^{l_w} y_w^s\, V_w^s T_w\left[\left(\sum_{c=1}^{3} F_w^c\right)\right]\right\} \qquad (1)$$

Where y_w^s is the binary decision variable; V_w^s is the substrate contribution of generator W_w (in L); T_w is the sludge toxicity level (dimensionless); F_w^c is the set of coefficients corresponding to the substrate composition (dimensionless). These coefficients are usually related to the content of organic matter, nitrogen and alkalinity and the equations used for such coefficients are tailored according to the case study. The objective of the cost function in regards to the case study is the maximisation of biogas production while optimising constraints related to nitrogen, alkalinity and the total volume of the digester. Thus, the coefficient related to organic matter shall increase at higher concentrations of organic matter (because the more organic matter, the more biogas produces the substrate); on the other hand, the coefficients related to nitrogen and alkalinity shall decrease as the concentration deviates from the optimum range.

However, an additional term is added to the correspondent cost function to consider logistics related to transport of each of the substrates selected as feed to digestion. Furthermore, it is attempted the same approach based on ACO to optimise simultaneously the feed of more than one anaerobic digestion system. Usually anaerobic digestion optimisation methods have been focused on optimising the feed of a single anaerobic digestion system at once; however, since the case study presents more than one WWTPs with anaerobic digestion, a simultaneous optimisation of all the anaerobic digestion receptors is attempted (while also including the aforementioned logistics factor into the cost function of the ACO algorithm).

$$B = 1/\left\{\sum_{w=1}^{N}\sum_{s=0}^{l_w} y_w^s\, V_w^s T_w \left[\left(\sum_{c=1}^{3} F_w^c\right)\rho_q + \frac{\rho_x}{X_w d_w I_w}\right]\right\}, \qquad (2)$$

Where ρ_q is the quality coefficient (dimensionless); ρ_x is the logistics coefficient (dimensionless); X_w is the unit cost (in €/km) of substrate transport; d_w is the distance between generator w and the anaerobic digester (in km); and $I_w = 1, \dots, 3$ is a coefficient related to the social impact of substrate transport (the higher the value of I_w, the higher the social impact of the related route).

The first term in the objective function in equation 2 aims to obtain the optimal characteristics of the anaerobic digestion input regarding different specifications of interest of this input e.g. toxicity, biogas production ability. Here, a novel second term is introduced taking into account the importance of the transport costs for anaerobic co-digestion of different types of sludge and industrial co-substrates. Specifically, this new term is related to the cost of the sludge/co-substrate transport, the distance between sludge/co-substrate generation and the corresponding digester —determined by the transport route—, and the social impact of this transport (depending on the routes considered). This proposal uses normalized values for the terms related to the quality and the transport. Also, the objective function in eq. 1 is constrained by the sludge/co-substrate characteristics —volume, composition, and toxicity level—, which are acceptable for the digester input in order to be suitable for the digestion process.

The cost function used is inspired by prior optimisation problems approached by the ACO algorithm such as in [47]. It is applied to optimise co-digestion strategies, but additionally taking into account the potential impact of the logistics associated with the transportation route of each co-substrate. The optimisation problem is solved by means of the ACO algorithm, which searches a solution using a probabilistic and iterative methodology. The specific procedure is an adaptation of the Max-Min Ant System [49], using an specific heuristic expression, shown in equation 3:

$$\eta_{ws} = \frac{V_w^s \sum_{c=1}^{3} F_w^c}{d_w} \qquad (3)$$

Hence, this is set as an optimisation problem which aims to find a solution towards favourable sludge/co-substrate characteristics and short distances/low social impact sludge/co-substrate transports. In addition, the algorithm implements mechanisms to avoid a rapid stagnation of the solution due to problem constraints. The proposed approach will be applied to the optimization problem of a real multi-plant case study, allowing the optimization of anaerobic digestion blends of 4 real WWTPs. These blends will be composed of: in-situ WWTP sludge, 12 ex-situ WWTPs sludge generators and 11 ex-situ industrial organic waste generators. The novel approach presented here considers both quality and logistics aspects of each waste contributor, providing an integral co-digestion planning strategy for a real multi-plant case study.

Optimisation of the cost function obtains a solution consisting of the contribution of each waste generator to the anaerobic digester, enabling logistic planning for centralized anaerobic digestion with the aforementioned sequence of waste contribution to the digester. Further calculations are made to show how the ACO algorithm enables obtaining a blend whilst respecting all restrictions set. These restrictions are primarily related to variables that are essential for proper control of anaerobic digestion: these variables are the carbon-nitrogen ratio, alkalinity and toxicity. The cost function also includes a term related to organic content so that the optimisation enables obtaining a blend with the highest organic content possible (and thus with the maximum possible biogas production).

Chapter Four

Case study

In this Chapter the case under study is presented through the following general topics related to problem analysis:

1. Description of the geographical context: the location specific context of the case study (and all their associated environmental, economic and societal conditions) must be determined to properly identify and be able to compare it with other cases around the globe without biases.

2. Analysis of currently implemented processes: an analysis of the current processes, performance of WWTPs and a mass balance and benchmark exercises are presented here.

3. Overview of sewage sludge management in CBT: a Strength-Weakness-Opportunities-Threats (SWOT) analysis is conducted to extract conclusions from the current state of the case study and point the untapped potential from the use of smart tools to improve the implementation process of waste valorisation in WWTPs.

4.1 Description of the geographical context

Before even starting to address the specific issues of the presented problem (sewage sludge valorisation in WWTPs) it is important to acquire an exhaustive perspective of the problem. The global context has already been introduced (the global resource crisis, the struggle for sustainability and the need for implementation of circular economy). That global context, coupled with the identification of the sanitation system as a particularly useful “political catalyst” to promote implementation of circular economy (since it is a WEF nexus), has led to conclude that sewage sludge valorisation is a promising strategy to further boost sustainability within the urban water cycle. Understanding the geographical context enables acquainting to which extent the anthropogenic impact on the region may condition eco-innovations such as the implementation of circular economy. That context is described according to the human-environment system concept. Combined, they compose the regional context and provide insight of its human-nature ecosystem.

The case study includes 23 WWTPs managed by *Consorci Besòs Tordera* (CBT), a public local water administration composed of 64 municipalities in four different regions of Catalonia (Spain) with a population of approximately 470,000 inhabitants. It is focused on the management of the sanitation system, the conservation of the river ecosystems and the promotion of environmental awareness to the general population.

The geographic location of the system corresponds to the upper parts of the Besòs and Rivers basins, across which the 23 WWTPs are distributed. Figure 8 shows the approximated location of each WWTP in the map.

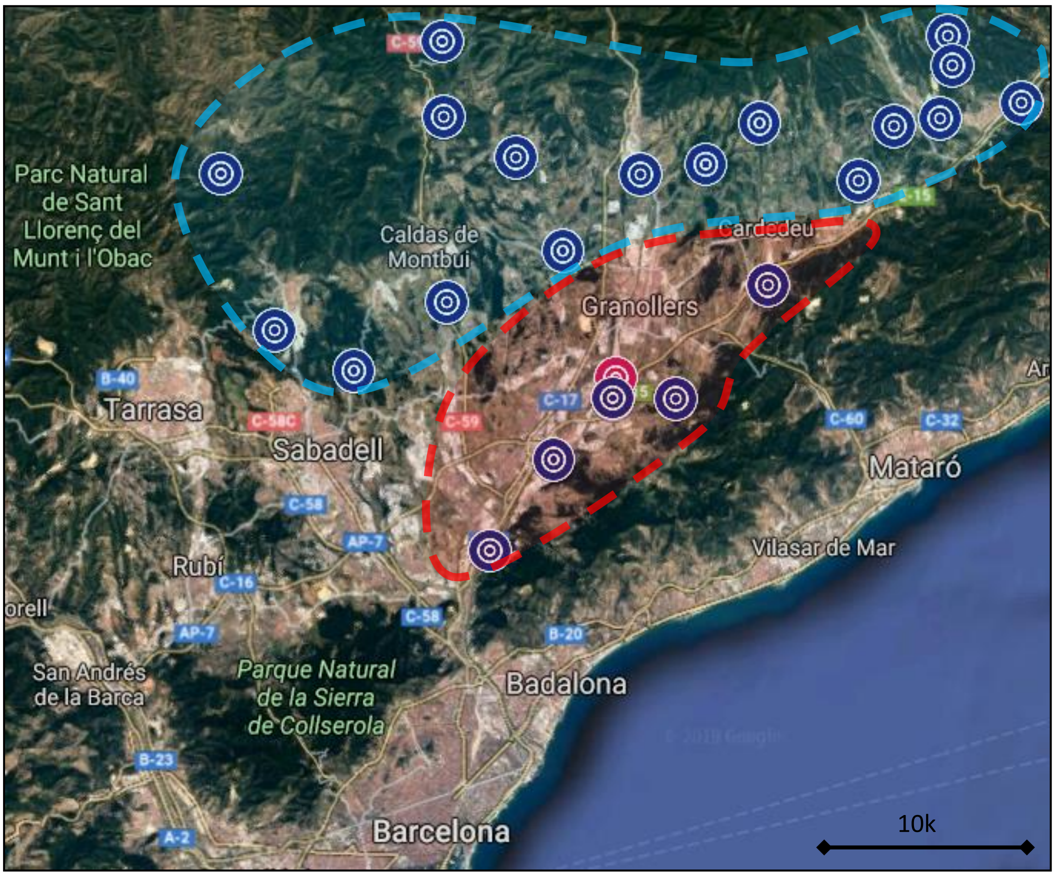

Figure 8. Map with the location of each WWTP of the sanitation system under study (dots). Blue shade indicates areas with low anthropogenic impact, and red shade indicates area with high anthropogenic impact. The studied sanitation system is comprised exclusively within these two areas (that correspond with upper parts of Besòs and Tordera river basins). The red-dotted WWTP corresponds to one of the most representative WWTPs, Granollers WWTP (that depurates wastewater from Granollers municipality cluster).

Regarding climate, it presents a Mediterranean biome, with relatively high temperatures and moderate to low precipitations (with high variations between years and relative unpredictability of yearly precipitation episodes and intensity). Thus, the system under study is relatively arid (or semi-arid). Considering the global context of climate change, forest fires are a significant risk for the region (and an actually increasing concern).

Water resources are relatively scarce, as in almost any territory with predominance of the Mediterranean biome. In fact, about a 60% of the Besòs river flowrate comes from the effluents of WWTPs [50]. Thus, WWTPs effluent must have as high quality as possible, which implies an additional challenge to optimise WWTPs performance. The unpredictability of precipitations, which allows the occurrence of some years of droughts, is the main reason behind both water scarcity and the potential risks of forest fires.

As for land use, the system under study is found basically around the *Vallès* valley (across which the river *Besòs* runs through). Relief is generally rugged in and out of such area and the bottom of the *Vallès* and outer valleys are mostly occupied by high-density settlements and a considerable network of roadways. Thus, agricultural activity is relatively low and fragmented through free spaces around the bottom of valleys. The other, more relief rugged areas around the valleys are relatively rural: although many low-density settlements and occasional agricultural areas can be found across, forest resources are the most abundant. No significant mining resources are found in the region.

The sanitation system under study is close to the metropolis of Barcelona. Although it is found downstream the river Besòs and, thus, it does not affect directly the wastewater collected in the WWTPs, the presence of the metropolis have a significant effect on the human activity of the *Vallès* valley: as the northern extension of Barcelona metropolis, the region under study has a high density of roadways, along which there are as well high density settlements (being *Granollers* municipality cluster the most iconic settlements of the system under study). Nevertheless, many low-density settlements can be found around the north and north-eastern areas of the system.

Regarding economic activity, there is a high degree of industrialisation bound to high density areas, and especially focused on chemical, pharmaceutical and agri-food manufacturing industry. As aforementioned in the environmental contextualisation, there are various agricultural areas, but they are a minor activity sector. And although there are high amounts of forest resources there is little forestry activity or woodworking industry. Aside from the services sector (which has little dependency on tourism due to the lack of great touristic attractions), the industry sector is the major economic activity of the area.

Overall, most of the system under study is highly populated, the main activity is related to the industry sector and there are high-density roadways. Considering the relative fragility of the described natural environment (affected by water scarcity, droughts and forest fires risk) it is concluded the anthropogenic impact on the region is very high. However, there are significant spatial heterogeneities, so that the outer areas of the system under study are considerable more rural: they have low-density settlements spread across the landscape along with agricultural areas, rich forestry resources and occasional agri-food industries.

4.2 Analysis of currently implemented processes

In this section a characterisation and benchmark process is performed for the WWTPs of the case study. For the purpose of benchmarking it has been used data from 252 European WWTPs (open-access data extracted from “Benchmark Database” from ENERWATER H2020 project webpage) and from 271 USA WWTPs (open-access data extracted from “Waste Survey Data” from Water Research Foundation webpage); these two databases, whose detailed source has been already indicated in the Chapter 3, will be mentioned from here on as “Europe WWTPs” and “USA WWTPs”, respectively.

4.2.1. By treatment capacity

Treatment capacity is a significant parameter to evaluate the case study: for instance, that can provide insight about the degree of centralization of wastewater treatment. That is an important issue because of the economies of scale: that is, the bigger the WWTP, the more economically feasible it will be to optimise its process and implement new ones; on the contrary, centralization of wastewater treatment in inadequate cases may imply a higher amount of investment on infrastructure to transport all the wastewater to the receiving WWTP. Figure 9 shows the 23 WWTPs of the case study organized according to its average flowrate. In Annex 1 it is shown the relationship of the WWTPs’ tags to their correspondent municipality.

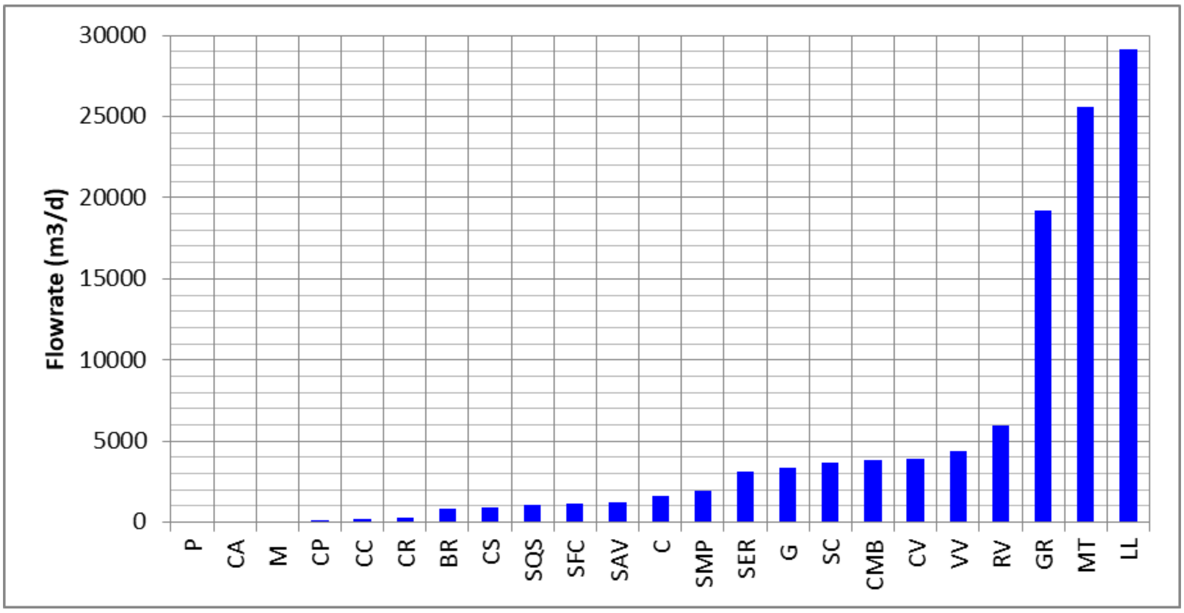

Figure 9. WWTPs of the case study (expresses as abbreviated tags) ordered by treatment capacity.

In comparison to WWTPs from Europe and USA, there is a higher portion of WWTPs from CBT below treatment capacities of 5000 m^3/day (83%, in comparison to 56% and 17% for the case of European and USA WWTPs). This means that wastewater treatment within the case study is more decentralized than average sanitation systems from Europe or USA. Thus, it supposes and additional challenge the implementation of innovative processes due to the reduced scales, and it may be expected a relatively lower performance for those WWTPs from CBT. Besides, for such relatively decentralized wastewater treatment systems centralization processes might be feasible strategies. Table 4 shows the percentage distribution of CBT, Europe and USA WWTPs.

Table 4. Proportion of WWTPs by treatment capacity range for the case study (CBT, data manually extracted from the cloud server database), Europa and USA.

Treatment capacity (m^3/d)	**WWTPs relative distribution**		
	CBT	**Europe**	**USA**
<5000	83%	56%	17%
5k-80k	17%	40%	73%
>80k	0%	5%	18%

Note that the aforementioned most representative WWTP of the CBT case study, *Granollers* municipality cluster WWTP (which corresponds to the tag “GR”) is not the WWTP with the highest treatment capacity, although it shares with LL and MT WWTPs the top three positions. Instead, another factor that influences the relevance of *Granollers* WWTP is the historical precedents of eco-innovation efforts carried in that municipality cluster (that will later be commented).

4.2.2. By nutrient removal performance

The most essential service that WWTPs provide with is the depuration of the three major macro pollutants: organic matter, nitrogen and phosphorous. Any of the three must be depurated from wastewater before returning to the river systems to avoid environmental pollution. However, the performance of the removal of such macro pollutants can vary considerably according to the strength of influent wastewater, temperature, the type of processes involved in the water line (especially in the biologic treatment) and the expertise of the operator of the WWTP. Table 5 shows a summary of the performance of WWTPs of CBT.

Table 5. CBT WWTPs (ordered from major to minor treatment capacity) average removal performance of carbon, nitrogen and phosphorous (in % removal from total of influent). Highlighted in green are the WWTPs that must meet a minimum effluent quality for the correspondent macro pollutant.

WWTP Tag	Macro pollutant removal percent of …		
	Organic Matter	Total Nitrogen	Total Phosphorous
LL	89	35	91
MT	94	82	94
GR	95	90	94
RV	90	87	84
VV	82	78	80
CV	95	84	88
CMB	94	87	82
SC	91	82	82
G	93	87	88
SER	94	91	88
SMP	95	84	73
C	91	87	61
SAV	94	92	58
SFC	93	92	80
SQS	95	93	84
CS	92	91	39
BR	87	55	80
CR	95	66	57
CC	86	63	27
CP	90	72	89
M	96	76	63
CA	90	66	29
P	96	62	65

Firstly, all WWTPs remove organic matter (through different biological processes all which are based on aeration). Mention is required to the fact that all the WWTPs from CBT that remove phosphorous do it through chemical precipitation (by addition of ferric chloride or similar reagents). However, only a 65% and 61% of the WWTPs of CBT depurate nitrogen and phosphorous, respectively. Both in European and USA WWTPs a 100% of WWTPs depurate organic matter (since it is the most basic water pollutant); but only a 31% of both of them depurate nitrogen, and a 24% and 18% of European and USA WWTPs depurate phosphorous, respectively. This means that WWTPs from CBT have to deal with higher restrictions on effluent quality, which is consistent with the previous observations about the sensitivity of the freshwater to pollution and the high anthropogenic impact on the regional environment of

CBT. In contrast, in Europe and USA there are a minor number of WWTPs that must deal with such effluent quality requirements, probably because their rivers have higher flow than those of CBT (Mediterranean biome with a context of water scarcity); thus these rivers would be more able to dilute the pollutants of WWTPs' effluents (and their anthropogenic impact might be lower, in consequence). Nevertheless, different regulations may apply across each case, so it would require a more exhaustive analysis. Table 6 shows the percent of WWTPs of each case that must accomplish macro pollutant removal.

Table 6. Proportion of WWTPs of CBT, Europa and USA that depurate organic matter, nitrogen and phosphorous.

	Proportion of WWTPs depurating		
	Organic Matter	**Total Nitrogen**	**Total Phosphorous**
CBT	100%	65%	61%
Europe	100%	31%	24%
EEUU	100%	31%	18%

Note that, despite the sensitive environment of the *Besòs* river basin, the WWTPs of low treatment capacity do not have obligation to fulfil nitrogen and phosphorous elimination requirements (see from BR WWTP downward in Table 5, which corresponds to a treatment capacity below 1000 m^3/day as shown in Figure 9).

4.2.3. By energy efficiency

Energy efficiency is an important variable that characterizes most of the WWTPs, especially because they allow reflecting the good quality and maintenance of the installations, and might allow highlighting the superior efficiency of some processes, or serving as a demonstration of the operators' expertise to optimise the WWTP performance.

A well-known way to compare energy efficiency is by plotting intensive energy consumption (per m^3 of influent wastewater) against the total inflow of the WWTP. That way it allows discerning the effects of economies of scale, that also affects energy efficiency: smaller plants are energetically less efficient, while bigger plants are more efficient (due to the fact that efforts to optimise are first put on the bigger plants because the economic impact on savings of these plants through energy savings can be potentially much higher than those of smaller WWTPs). Figure 10 shows a plot of energy efficiency for CBT; Europe and USA WWTPs.

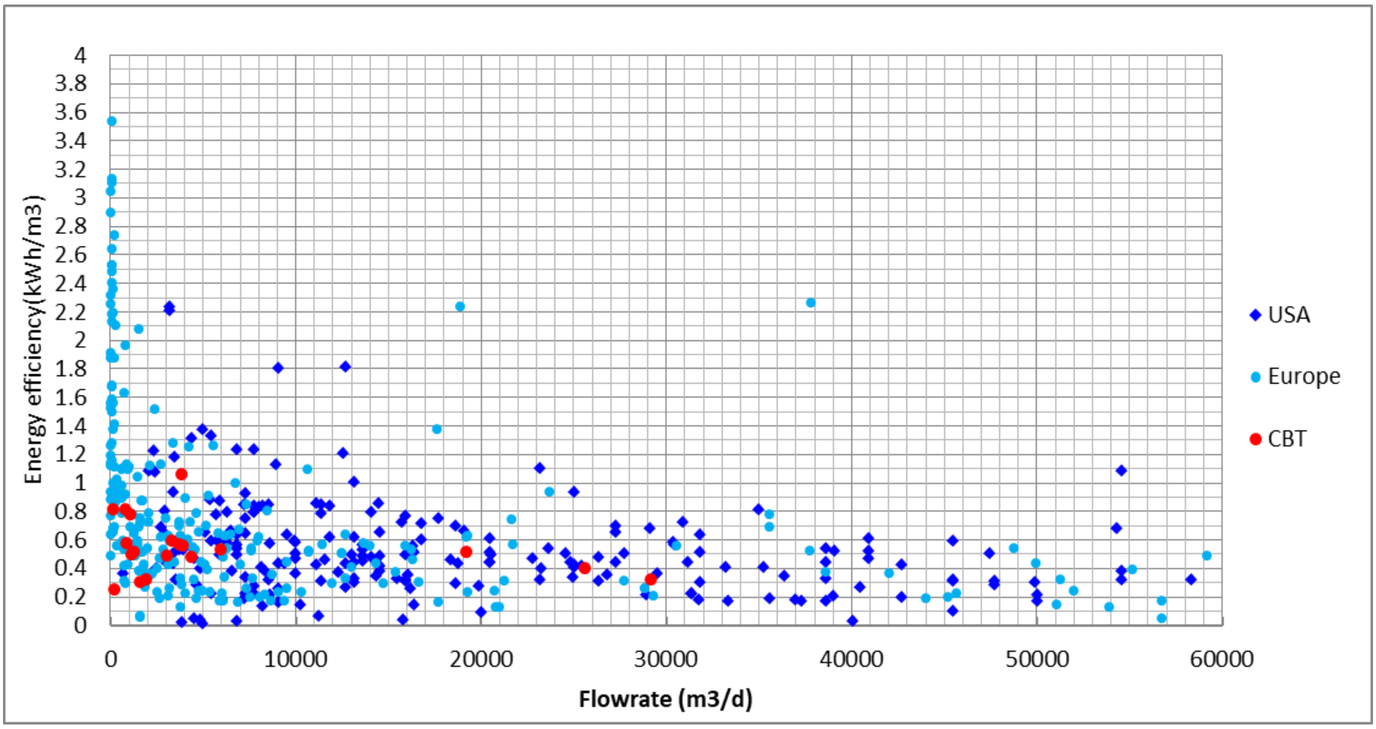

Figure 10. Energy efficiency plot of CBT, Europe and USA WWTPs.

As previously stated, it is confirmed for all three cases (CBT; Europe and USA WWTPs) that the smaller the WWTPs the lowest the energy efficiency (that is, the highest the intensive energy consumption). This trend is especially pronounced for WWTPs below 1000 m^3/day, and an increase of flowrate has associated a decrease of energy efficiency in the form a curve with decreasing steeps: thus, energy efficiency in the range of 1000-10000 m^3/day to an approximate average of 0.45 kWh/m^3 and for major treatment capacities energy efficiency is only slightly reduced, up to 0.2-0.3 kWh/m^3. Also note that smaller WWTPs have a high variability of energy efficiencies, while bigger WWTPs presents lower variability: the reason behind this trend is that smaller WWTPs have a major variety of process configurations, modes of operation and optimisation strategies, but there is no definitive solution, so each one adopts different strategies; instead, for bigger WWTPs there are established relatively common technologies and strategies of energy-optimisation, so the options are more reduced and, thus, there is lesser variability for higher flow WWTPs. In [51] the effect of the technology configuration of WWTPs on the energy efficiency is discussed with detail.

As for CBT WWTPs, a qualitative analysis shows that they are generally located between the centre and bottom areas of the energy efficiency in Figure 10 of both Europe and USA. Thus, it can be extracted, as a general trend, that CBT WWTPs are slightly more energy efficient than average Europe and USA WWTPs.

4.2.4. By sewage sludge management processes

The sewage sludge line has the main function of reducing the volume of sewage sludge produced (by extracting its water) and, if possible, sanitize it (through processes as anaerobic digestion). However, not all the sludge lines are always the same; the 23 CBT WWTPs can be classified in four groups according to the configuration of their correspondent sewage sludge lines:

1. WWTPs that do not have any sludge line process (not even the first process of thickening): WWTPs BR, CC, CA and M instead of having implemented a sewage sludge line of their own they have a collector that sends continuously the sewage sludge produced down to another WWTP with a complete sewage sludge line.

2. WWTPs with a partial sludge line: that is the case of WWTPs P, CA and CR, that only have a thickening process. The thickened sewage sludge is accumulated in that reactor, and a tank truck comes often to collect it and discharge to a WWTP with a complete sewage sludge line. Overall, these type of WWTPs are similar to group 1, but sludge transport is discontinuous instead.

3. WWTPs with a complete sewage sludge line without anaerobic digestion: these WWTPs (the 12 CBT WWTPs found between VV and CS WWTPs corresponding to Table 5) have sludge thickening followed by dewatering, but no further processes. Thus, the sludge cake produced is not sanitized.

4. WWTPs with a complete sewage sludge line and with anaerobic digestion: the four biggest WWTPs from the CBT system (LL, MT, GR and RV) have sludge lines of thickening, mesophilic anaerobic digestion and dewatering. The sludge cake they produce is relatively sanitized (although it is not considered class A biosolids) and there is an additional process line to store and process the produced biogas: the biogas line is composed of gasometers, a cogeneration system (to produce electricity and heat from the biogas) and a torch (to burn the excess biogas that can't be valorised).

As observed by comparison of the previously used databases for benchmarking, Europe and USA WWTPs have about a 40% and 45% of WWTPs with anaerobic digestion, respectively. In contrast, a 19% of CBT WWTPs have this process. The main reason behind is that economies of scale play a significant role in the implementation of anaerobic digestion: these processes require a solid (and expensive) infrastructure, so it is only affordable for relatively big WWTPs (such as LL, MT, GR and RV WWTPs). Also, different codigestion activities have been performed at GR and MT WWTPs, specifically with high strength substrates; however, no optimisation tools are applied, so the substrate dosage is kept below its potential to avoid over dosage risk.

Currently, the codigestion processes are based on manual demand and delivery of substrates by decision of the practitioners according to their evaluation of the anaerobic digester operation performance. However, the use of optimisation tools would improve significantly the current codigestion process by enhancing the dosage strategy and serving as an additional support tool for practitioners in charge of the quality control. Furthermore, the use of such optimisation tools as the one developed in this thesis allows maximisation of the blend addition while assuring safe limits of operation via data monitoring. Thus, here relies a key contribution of the thesis to the challenge of centralized co-digestion, where key issues are usually the high complexity of the setting (tackled via the use of a smart tool that processes all datasets of each substrate), and the co-existence of multiple constraints (tackled via the ACO-based method optimisation that maximises biogas production while adjusting the concentration of key compounds such as nitrogen and alkalinity and minimising metal toxicity).

Regarding the management of the sludge cake produced at the end of the sludge line (after dewatering), the disposal ways of application are similar to those of organic wastes of low environmental hazards, and since it achieves a solid consistency its handling is relatively easier when compared to liquid sewage sludge. The different disposal ways are as follows:

1. Landfill: this has been a conventional disposal way during the last decades; however, it has a high environmental impact and it’s becoming increasingly expensive (due to environmental policy taxes to discourage that disposal way). As a result, this is a last resource.

2. Composting (and other biological treatments to sanitize sludge and convert it to agricultural fertilizer): in the CBT region this is a common way for those sludge cakes that are not sanitized enough within the WWTPs to be directly used as agricultural fertilizers (such as the disposal way 4.); once sanitized in composting plants or similar infrastructures, the remnants sludge cake is used as agricultural fertilizer (in the same fashion that disposal way 4.). As previously mentioned, economies of scale impair significantly the implementation of sanitizing infrastructure for most WWTPs (such as anaerobic digestion), so most of them lack sanitizing processes and must send sewage

sludge to composting. However, this trend also applies for most organic waste generators across the region; consequently, the existing composting plants are being overloaded with organic wastes, and disposal prices have been rising significantly during the last years in Catalonia. Thus, the economic feasibility of this disposal way is decreasing over time.

3. Thermal valorisation, also called waste-to-energy (including drying, cement kilns and other variations of processes involving the use of high temperatures to extract value from sludge): since sludge has a significant amount of organic matter, it can be oxidized to produce energy. That is the basis of this disposal pathway, which revolves around energy-intensive processes, usually involving the use of sludge as fuel to obtain thermal energy (such as cement kilns or directly power plants). Usually (along the last decades) these processes have carried low public acceptance due to the inherent risks of accidents related to the handling of energy-intensive processes; nevertheless, during the last years waste-to-energy has emerged as an attractive way to increase energy availability. Indeed, that disposal way contributes to ameliorate the energy crisis, as well as reducing total waste to be handled to ashes; on the other hand, such ashes must be additionally handled as a new waste (which has a variety of options including landfill as the most common – due to the high concentration of metals invalidating other options –, or use as a fertilizer component for specific cases). Besides, the sludge combustion generates significant emissions that require additional filtering and carbon-sequestration processes to reduce the impact of such emissions. Even in the case that the impact of ash management and emissions would be reduced effectively, the high costs associated to the implementation of the whole process is significantly high, so its economic feasibility, although viable (due to the potential revenues generated by energy generation) requires high amounts of capital inversion (whose lack is precisely is one of the greatest bottlenecks of implementation). Nevertheless, there exists a synergism between thermal valorisation of sewage sludge and the forestry sector: the combination of both wood fuel and sewage sludge is a potentially feasible strategy that may help improve economic feasibility while promoting the regional forestry sector.

4. Direct use as agricultural fertilizer: this disposal way currently is the most accepted, because of its potential to replace mineral fertilizers (a direct benefit to the agricultural sector and to its value chains) and its affinity for the circular economy

concept. Thus, this disposal way allows sustainability implementation on the rural areas, which comprehend a significant part of the case study of CBT and of Europe in general. However, microbial and metal-related risks are a major concern when using sludge as a fertilizer, so legislation regarding fertiliser quality is becoming increasingly restrictive: only the best quality of sludge, free from pathogens, metal content and even micropollutants should be used as fertilizer; this implies that most organic wastes wouldn’t be able to serve as fertilizer without being treated via additional processes (which carry their respective economic burden, especially in those cases where it isn’t yet implemented). Overall, sewage sludge quality requirements (for fertiliser disposal) are increasing over time; for example, if sewage sludge hygienization requirements increase, WWTPs with mesophilic anaerobic digestion will not be able to meet the new standards and shall implement technologies that allow achieving 55ºC along the process (such as thermophilic anaerobic digestion or thermal hydrolysis) to keep business of sewage sludge management as usual. Otherwise, either composting (which has a decreasing feasibility due to overloading of plants and disposal price increase) or thermal valorisation (that is becoming a favoured disposal pathway) would be the next prioritized disposal paths.

4.2.5. By mass balances

Mass-balances are a well-known tool to assess the performance of WWTPs, especially from a wide plant perspective that can integrate all the inputs and outputs. The characterisation of mass balances improves the understanding on how different technology configurations affect the distribution of outputs (for example, how much does anaerobic digestion contributes to transforming influent organic matter into energy carriers as biogas). Thus, in

For all CBT WWTPs mass balances have been calculated based on the use of routine measurements of all inputs and outputs of the WWTP: mass-balance calculations are performed for elemental carbon and elemental nitrogen. Inputs and outputs for each mass-balance flows are independently solved (5 and 4 flows for carbon and nitrogen, respectively). Table 7 and Table 8 summarise carbon and nitrogen flow calculation main features, including data and constants required. Note that the liquor returns from the sludge line are not included (since it is a recirculating flow within the WWTP).

Table 7. Summary of elemental carbon mass-balance flows and data calculation. Whereas COD-Chemical Oxygen Demand ; BOD-Biochemical Oxygen Demand ; %CH4,%CO2-Volume fractions of CH4 and CO2 in biogas; P-Biogas Pressure ;T-Biogas Temperature; R-ideal gas constant; SM-Solid Matter (%) ; SVM-Solid Volatile Matter (% on SM) ; COD to C stoichiometric conversion = 0,375gC/gDQO ; ratio CO2/BOD removed=0,7gCO2/gBOD removed (extracted from Khiewhijit et al (2015)) ; CO2 to C stoichiometric conversion = 0,27gC/gCO2 ; CH4 to C stoichiometric conversion = 0,75gC/gCH4 ; SVM to C stoichiometric conversion = 0,53gC/gSVM (factors extracted from [52,53]**)**

Flow ID	**Flow description**	**Data used for calculation *(% error, if known)***
C1	Influent Carbon	Flow (*5%*) ; COD (*16%*) ; COD to C stoichiometric conversion
C2	Effluent Carbon	Flow *(5%)* ; COD *(16%)* ; COD to C stoichiometric conversion
C3	CO2 emitted from biologic reactor	Flow *(5%)* ; BOD removed *(18%)* ; Ratio CO2/BOD removed ; CO2 to C stoichiometric conversion
C4	Biogas Carbon	Flow *(5%)* ; %CH4 ; P ; R ; T ; CH4 to C stoichiometric conversion ; %CO2 ; CO2 to C stoichiometric conversion
C5	Output sludge Carbon	Flow ; SM *(5%)* ; SVM *(5%)* ; SVM to C stoichiometric conversion

Table 8. Summary of elemental nitrogen mass-balance flows and data calculation. Whereas TN-Total Nitrogen; NH4+-Ammonia; SVM to N stoichiometric conversion = 0,124gN/gSVM (factors extracted from [52,53]).

Flow ID	**Flow description**	**Data used for calculation *(% error, if known)***
N1	Influent Nitrogen	Flow *(5%)* ; TN *(15%)*
N2	Effluent Nitrogen	Flow *(5%)* ; TN *(15%)*
N3	N2 emitted from biologic reactor	Flow *(5%)* ; NH4+ *(12%)*
N4	Output sludge Nitrogen	Flow ; SM *(5%)* ; SVM *(5%)* ; SVM to N stoichiometric conversion

An approach for phosphorous elemental mass-balance was attempted, but no consistent daily data was available for output calculation. Hence, no phosphorous elemental mass-balances are performed in the context of this study. In Annex 2 it is shown the summary of data used to characterize all carbon and nitrogen mass-balances in relation to the WWTP diagram and the equations used to estimate each carbon and nitrogen mass-balance flow are described.

The methodology for mass-balance calculation is based on classical rules of input-output balance computation [34] where the input-output gap is expressed as percentage of influent carbon or nitrogen. Besides, all uncertainties associated to measurements were quantified, and uncertainty propagation is calculated for i) the process of flow calculation and ii) the global input-output subtraction, by usual expressions of error propagation, as used in [54]. Total uncertainty is calculated as an absolute value for each balance performed. However, it is expressed as percentage of influent carbon or nitrogen, and it is compared to the percentage gap of input-output for its correspondent mass-balance. When total uncertainty is higher than the mass-balance gap (both expressed as percentage of the influent carbon or nitrogen), it is considered that the zero-gap is within the range of uncertainty of the calculus. Hence, in these cases the mass-balances are fitted under the uncertainty range and, thus, considered as “a closed mass-balance” (since uncertainty propagation enables explanation of the input-output gap).

A complete summary of elemental carbon and nitrogen mass-balances results are given for each of the 23 WWTPs under study in Table 9. For the carbon mass-balances, 14 out of 23 are fitted under their uncertainty range, and 22 out of 23 nitrogen mass-balances are fitted under their respective uncertainty range. This means that for most WWTPs the input-output gap generated by the mass-balances calculation can be explained by propagated uncertainty.

Table 9. Summary for elemental carbon and nitrogen mass-balance fitting under uncertainty range. The carbon and nitrogen gaps refer to the input-output gap, expressed as percentage over influent carbon or nitrogen content, respectively. WWTPs are sorted from higher to lower daily wastewater treated.

WWTP ID	Average flow (m3/d)	Elemental Carbon Mass-Balance Fitting			Elemental Nitrogen Mass-Balance Fitting		
		C balance gap (%)	C balance propagated uncertainty (%)	Fitted under uncertainty range?	N balance gap (%)	N balance propagated uncertainty (%)	Fitted under uncertainty range?
LL	29200	10,9	29	Yes	10,5	28	Yes
MT	25700	22,1	27	Yes	3,9	27	Yes
GR	19300	21,5	27	Yes	8,1	26	Yes
RV	6000	25,6	27	Yes	1,1	27	Yes
VV	4400	21,8	28	Yes	3,2	27	Yes
CV	4000	24,2	27	Yes	23,5	29	Yes
CMB	3900	11,8	29	Yes	13,4	28	Yes
SC	3700	57,1	23	No	3,9	27	Yes
G	3400	5,9	31	Yes	11,6	28	Yes
SER	3100	10,0	28	Yes	6,1	27	Yes
SMP	2000	31,6	27	No	7,2	28	Yes
C	1700	30,2	27	No	10,3	26	Yes
SAV	1300	35,1	26	No	1,3	27	Yes
SFC	1200	23,3	27	Yes	9,2	25	Yes
SQS	1100	8,0	29	Yes	24,7	27	Yes
CS	910	24,8	28	Yes	10,0	26	Yes
BR	850	115,4	26	No	41,7	24	No
CR	250	76,0	21	No	16,8	27	Yes
CC	200	55,6	27	No	8,9	22	Yes
CP	150	64,3	23	No	3,2	28	Yes
M	80	71,5	24	No	25,8	32	Yes
CA	60	51,4	26	No	10,9	30	Yes
P	40	20,2	23	Yes	3,0	25	Yes

The first highlight is the uncertainty source of the model: as shown in Table 7 and Table 8, the major uncertainty source comes from determinations of COD, BOD, TN and Ammonia (acquainting for errors of 16, 18, 15 and 12%, respectively). These are measurements made by laboratory assay with ISO 17025 (from the daily quality control of WWTPs). The acquainted errors are established by the method standards. This means that even the Best Available Techniques for wastewater determination (which are those that are implemented for ISO 17025 laboratories) have a significant uncertainty source. There are also relatively minor uncertainty sources coming from flow measurements and SM and SVM content determination (all of them aquatinting for about a 5% estimated error, according to operators' procedures and internal protocols). Those uncertainty sources, along with traditional uncertainty propagation rules, may help to explain why the total carbon and nitrogen mass-balances uncertainties have values about 20-30%.

Figure 11 shows elemental carbon and nitrogen fraction distributions amongst all the output vectors for each WWTP. Note that distributions are expresses as percent relative to the total of the balance itself, without further considering uncertainties that have been discussed previously. Besides, for the 7 smaller WWTPs (BR, CR, CC, CP, M, CA and P) inconsistent data was found regarding sludge output measurement and thus are not included.

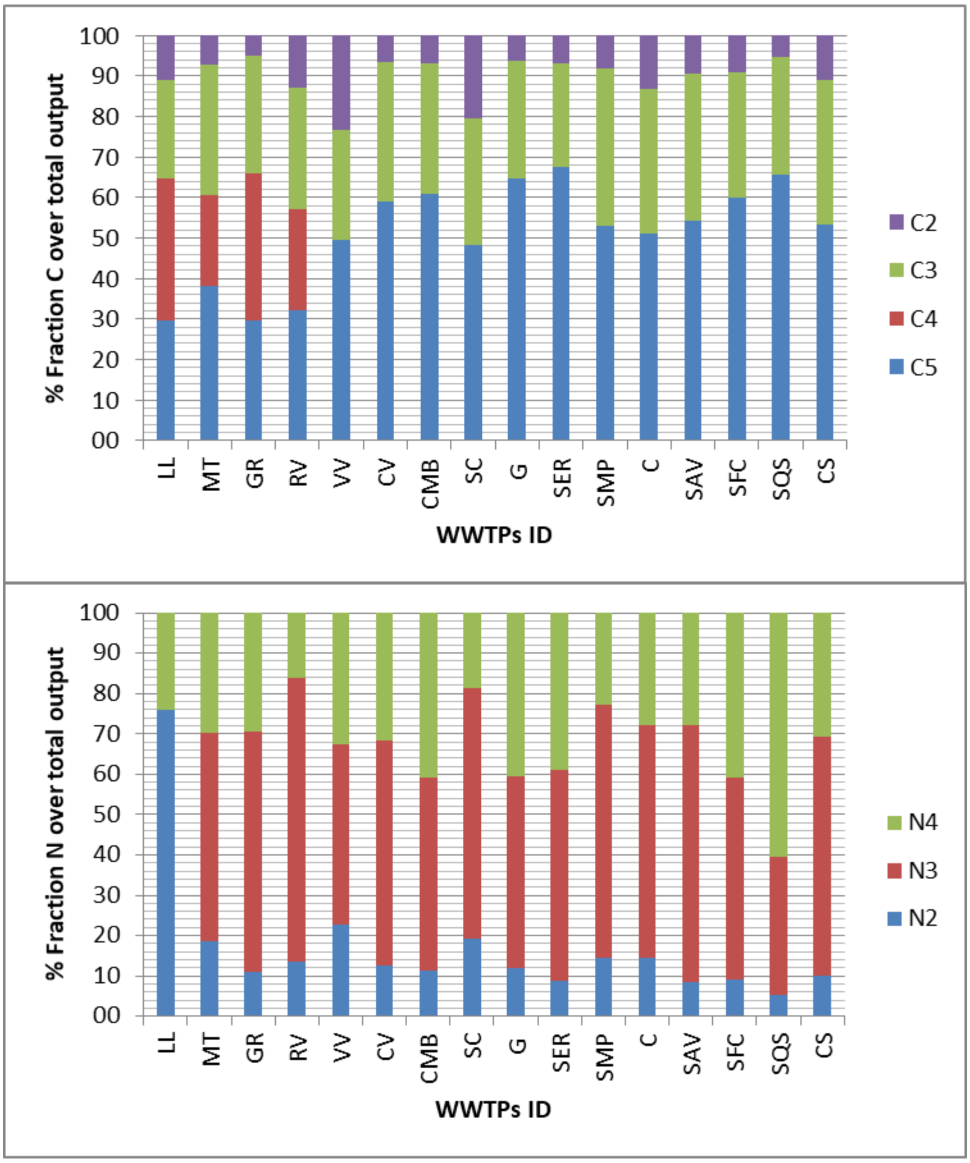

Figure 11. Elemental carbon (top) and nitrogen (bottom) mass-balance fractions distribution for each output vector for CBT WWTPs (organized by descending average flow treatment from left to right).

Only the four bigger ones have anaerobic digestion in the sludge line (i.e. WWTPs LL, MT, GR and RV). This results in a 30% of output carbon being converted to biogas (flow C4) and about another 30% of carbon output being concentrated in sludge (C5); for the rest of WWTPs, about a 60% of carbon output would be concentrated in sludge. On the other hand, all WWTP except LL (precisely the biggest one) perform nitrification, which results in about a 50% of output N being emitted as N2 through biologic reactor; and, if anaerobic digestion is present, seems that nitrogen content of sludge slightly reduces (from 24-44% for WWTPs without anaerobic digestion and 18-30% for WWTPs with anaerobic digestion, including LL WWTP). Within the 4 WWTPs with anaerobic digestion, is interesting to note that sludge nitrogen content (after anaerobic digestion) does not present clear differences between LL (the only one without nitrification) and GR, MT, RV WWTPs.

These results confirm the high potential of anaerobic digestion processes to valorise half of sludge organic content into biogas. Besides, consistence of the results for each WWTP is appreciated, implying that the applied method for mass-balance calculations can be replicated with confidence for different WWTPs.

The performed mass-balances are compared to previous work on elemental mass-balance found in the literature. Relative distribution fractions of the following output carbon are the object of comparison: C3 (biologic reactor emissions due to organic matter oxidation); C4 (biogas production if there is anaerobic digestion in the WWTP); and C5 (sludge organic matter content, produced at the end of the sludge line). The same comparative process is applied for nitrogen mass-balance, where the output vectors N3 (biologic reactor emissions coming from nitrification) and N4 (sludge nitrogen content, produced at the end of the sludge line). Table 10 compares the results of the present study to homologous data from previous works on elemental mass balance modelling of WWTPs [34,52,55,56].

Percentage distribution for each carbon and nitrogen output was similar to ratios established by previous works on elemental mass balance found in the literature. Most of the literature reference values are inside or near the range established in the framework of the present study: take for example carbon output through biogas vector, where the present study framework establishes a range of 23-37% and reference values account for 29, 39 and 34%, respectively. However, some reference values shall be compared and discussed according to the processes for each case, and uncertainty for the literature mass-balances shall be conducted (although it is not available in the correspondent works) in order to assess whether their associated uncertainty is similar to that of the herein presented approach.

Table 10. Comparison of the mass-balance approach calculation with raw operators ‘data and literature data on elemental carbon and nitrogen mass balance modelling within WWTPs. Results for the present study are expressed as an average ± standard deviation of the study ’set WWTPs with and without anaerobic digestion (expressed as AD).

Reference	**This study**		**Fernández-Arévalo et al (2017a)**	**Gans et al (2010)**	**Khiewhijit et al (2015)**	**Carlsson et al (2016)**
Methodology	Independent flow solving		Plant Wide Modelling Simulation	Theoretical factor conversion	Theoretical factor conversion	Theoretical factor conversion
Input data	Flow-specific daily operation measurements		Influent-effluent data	Literature data	Sampling campaign (4 points)	Influent-effluent data
ELEMENTAL CARBON BALANCE						
Input-Output Gap (%)	22 ± 13,5		0	0	0	0
Uncertainty (%error)	26 ± 2,4		?	?	?	?
%Fraction C output sludge	32 ± 4,0 if AD 57 ± 6,5 if no AD		31 (with AD)	20 (with AD)	27 (with AD)	33 (with AD)
%Fraction C output biologic reactor CO2	31 ± 4,0		33	6	35	36
%Fraction C output biogas	30 ± 6,9 if AD 0 if no AD		29 (with AD)	39 (with AD)	34 (with AD)	?
ELEMENTAL NITROGEN BALANCE						
Input-Output Gap (%)	9 ± 6,9		0	0	0	0
Uncertainty (%error)	27± 2,0		-	-	-	-
%Fraction N output sludge	24 ± 6,3 if AD 34 ± 10,9 if no AD		25	5	14	39
%Fraction N output biologic reactor N2	51 ± 16,1		58	76	48	15

Usually elemental mass-balance modelling heavily relies on model calibration and validation. In [55] theoretical mass-balances of Gaobeidian WWTP were performed, using literature theoretical conversion factors with measured data obtained in a two-month sampling campaign. In [52] mass balances were performed based on a data set comprised of the influent quality of 29 Dutch WWTPs and empirical, laboratory-scale proven, conversion and efficiency factors (which were used to estimate all the output vectors of the WWTPs from the influent data). In [56] there were combined both experimental data and theoretical assumptions; [34] applied a self-developed method, the Plant-Wide Modelling (whose main features can be found in [57] to calculate mass-balances; however, these are calculated by influent and effluent data, while the other output vectors (such as sludge, emissions or biogas) are estimated using complex model-based conversions. Despite they achieve to close mass balances, none of these previous works on mass-balance assesses the uncertainty associated to the model or its input data, which is crucial to provide new-generation reliable models [58]. Besides, input data of the aforementioned models is related basically to influent and/or effluent data, flow-balance assumptions and stationary-state dynamics; or, otherwise, costly analysis campaigns. However, the mass balances performed for the 23 CBT WWTPs have been performed by independently calculating each input and output of the plant (that is, using different variables for each one), which has allowed to reassure previous results observed on bibliography and to estimate propagated uncertainties from the balance. Comparing the propagated uncertainty with the mass-balance gap has allowed assessing how “closed” could be considered each mass-balance.

The results from these mass balances prove the effectiveness of anaerobic digestion in the conversion of organic matter in biogas, as well as considering the weight of sludge disposal in regard to the total fraction of carbon and nitrogen that it carries. Besides, carrying on the mass balances on the WWTPs of the case study helps understand the state of their processes and allows further benchmarking exercises amongst them or with other external WWTPs (which was the purpose of this section).

4.3. Overview of sewage sludge management in CBT: SWOT analysis

A SWOT analysis is performed to summarize the current state of sewage sludge management in the CBT, as shown in Table 11, considering that the objective to achieve in the case study is implementation of optimal sewage sludge management.

Table 11. SWOT analysis of sewage sludge management in CBT. The objective of the case study is implementation of optimal sewage sludge management.

	Helpful To achieve the objective	**Harmful** To achieve the objective
Internal origin (CBT system and WWTPs related issues)	**STRENGTHS**	**WEAKNESSES**
	1. CBT WWTPs performance is slightly over the average of European and USA WWTPs (of similar size) 2. The biggest WWTPs already have anaerobic digestion 3. Although the smaller WWTPs haven't anaerobic digestion, they are relatively close to WWTPs with anaerobic digesters 4. Communication between public administrations is relatively fluid	1. Lack of on-line data monitoring centralized infrastructure 2. Lack of a knowledge management system to facilitate knowledge and experience transference between internal actors 3. Lack of smart tools to aid in quickly adaptation of WWTPs to new utility management conditions 4. Lack of advanced processes to increase sludge or biogas quality
External origin (global and regional context related issues)	**OPPORTUNITIES**	**THREATS**
	1. Sanitation has a key role in achieving sustainability 2. Sewage sludge valorisation is directly linked to circular economy 3. Synergies are possible with external industrial organic wastes (for codigestion) 4. Synergies are possible with the forestry sector (for combined sewage sludge and wood fuel thermal valorisation) 5. Much knowledge is available (from professional associations, conferences) to further boost implementation of new processes	1. The global resource crisis 2. Lack of funding sources for infrastructure maintenance and implementation of new processes 3. Lack of adaptability to quick policy changes 4. Increasing anthropogenic impact (due to urban development) 5. Sensitive environment and climate change 6. Since eco-innovation involves actors across sectors, its implementation can be impaired by the lack of willpower of only a few actors across the new value chain to be implemented

Overall, strengths of the current status of sewage sludge managements in the case study favour the implementation of centralized anaerobic digestion, and remark the relatively good performance of the WWTPs. Weaknesses are focused on the lack of smart tools to improve the implementation (and eco-innovation) processes. Supplying these tools may grant a chance to exploit the various opportunities presented in the regional context (the high amount of knowledge, waste synergies and the chance to contribute to sustainability within the plant and within the sanitation system as a whole). Accomplishing these milestones (weakness counteracting and, after that, opportunity exploitation) would enable an increase of resilience to face the various threats presented. Thus, developing smart tools designed to exploit the present opportunities (which mainly revolve around waste synergy and knowledge and data availability) is a priority to increase the resilience of sanitation systems.

Chapter Five

Implementation of a Decision Support System for Sewage Sludge Management

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5.1 Introduction

The paradigm shift from a linear to a circular economy represents an opportunity to address different emerging challenges of the 21st century regarding various aspects derived from population growth and resource scarcity (in terms of water, energy or even food) as well as the need to transition to a low-carbon economy [8].

Since WWTPs are a water-waste-energy nexus and are a fundamental pillar of sustainable development, they play a key role in the implementation of a circular economy. Furthermore, proper development planning for future WWTPs that is coupled with sustainable solutions is an increasing concern. Currently, a paradigm shift is taking place from the concept of "wastewater treatment plants" to "water resource recovery facilities" (WRRFs), and increasing interest in next-generation modelling for circular economy related processes has been observed [16,34,59]. Specifically, processes related to sewage waste valorisation and energy generation (e.g., anaerobic digestion and biogas production) are major issues to be addressed [26,60].

However, socio-environmental challenges regarding circular economy implementation are becoming a major concern. Conventional methods of information gathering and processing to properly justify decision-making are becoming highly time-and resource-consuming. Hence, new methods of assessing decision-making processes are required to meet current challenges, such as the rapidly changing environment [58].

On the one hand, simulation software allows the estimation of the output of the problem by varying the process configuration and the input data (hence providing a general framework for the creation of study cases). Simulation-based methods are convenient for representing the behaviour of a real system for further purposes, e.g., fault diagnosis [61], but validated actual data and a good knowledge of the actual system are required to obtain reliable results. Usually, the output of these processes is summarized in key performance indicators (KPIs). Some examples of modelling practices for WWTPs include energy and mass balance simulation – see, e.g., [34,56,62,63] – and economic assessment together with viability analysis as presented in [24]. However, employing these approaches is resource- and time-consuming, so new, more integrated and automated methods are required for future WWTP planning. Further work is also required to assess the impacts of new technologies and different configurations, develop real case studies and address the uncertainties associated with each scenario.

On the other hand, decision support systems (DSSs) enhance the decision-making process and allow a higher degree of complex problem solving from a more holistic perspective that usually includes environmental and economic assessments. Examples of the application of DSSs to optimize decision-making regarding WWTPs can be found in recent literature, e.g., [64,65]. In addition, DSSs are being developed and validated for specific processes in WWTPs, as in [35], where a DSS was developed to optimize the operation of a biogas upgrading facility. In regard to regional-level planning and management, DSSs may be supplemented with further simulation or algorithm-based methods, e.g., in [9], where KPI-based models were developed to evaluate the performance of different worldwide circular economy implementation projects on a large-scale basis. Additionally, in [66], a specific network of waste-to-energy pathways was designed and optimized for waste- and biomass-sourced energy carriers. Hence, DSSs have been proven to be useful for process- and plant-level decision-making. In addition, simulation-based methods are interesting for performing studies at the regional level.

In recent years, different projects have been conducted to enhance WWTPs development and demonstrate their achievements with simulation models and pilot plants – see, e.g., [67,68] – and have also included different user-adapted DSS tools as a means to compare and highlight the added value of the proposed technologies. Since both simulation- and DSS-based procedures have the potential to overcome challenges in circular economy implementation, DSS coupled with plant simulation is a promising strategy for providing holistic insights from the technical to the strategic levels of decision-making. However, there is a lack of available solutions that fully merge simulation and DSS methods for WWTP planning (mainly due to the lack of available case-study data to carry out extensive simulation and validation studies).

Thus, there is a need for innovative tools to provide assessments of potential technology implementation in WWTPs in order to facilitate their transition towards more sustainable processes. The authors propose and validate such a tool here. The focus has been placed on the implementation of processes related to the sewage sludge line due to their relevance to the circular economy transition. Some studies have focused on WWTP water line technology assessments – see, e.g., [59,69] – and there is also increasing interest in the implementation of the circular economy, where WWTP waste management plays a key role. Aside from anaerobic digestion, which is a widely implemented process, other well-known processes that enhance sewage sludge treatment include thermal hydrolysis, which, in turn, sanitizes sludge, allowing it to become a class A biosolid according to the Environmental Protection Agency (EPA) [25] and increases anaerobic digestion biogas production; and drying followed by thermal valorisation of the final sludge cake, which allows a substantial reduction in waste production and increases energy recovery (which is usually consumed in the prior drying process). Although these processes are well known, there is still a lack of tools to provide holistic assessments of the combination of sewage sludge processing technologies.

Hence, the objective of this paper is to develop and validate with real case-study data a WWTP simulator coupled with a DSS and to use a hierarchical KPI approach to the case-study assessment focused on sewage sludge valorisation processes. The combination of these methods will allow extended and automated performance studies of the different strategies for sludge management and their corresponding technology configurations in real case studies. This will provide a substantial enhancement to the decision-making process for optimum circular economy strategy implementation through the selection of the best-fitting sewage sludge valorisation strategies and will also improve the management of all the required decision-making data of the whole wastewater treatment system under study.

5.2 Materials and methods

In [65], a comprehensive guide to DSS design can be found. The usual steps of DSS development are as follows: 1) problem analysis (i.e., stating the objective and both the conceptual and the physical system frameworks); 2) data and knowledge acquisition; 3) cognitive analysis; 4) model selection; and 5) model implementation.

5.2.1 Problem analysis

Regarding problem analysis, four tasks must be performed: a) determine the objective of the tool; b) determine what data are required for input into the tool; c) determine what data are available from the system under study; and d) determine what procedures are required to fulfil the objective based on the available data and their properties (these are generic methods only and will later be the foundation for model selection and implementation).

The objective of the tool presented here is to provide an assessment of sewage sludge valorisation processes in a real sanitation system). The data required for the assessment are time-series of KPIs designed ad hoc by the authors (and based on common drivers of the wastewater sector) for the wastewater sector, with a focus on waste and asset management aspects [70,71]. Data on the mass, energy, nutrient, GHG emissions and economic balances are needed, and parameter estimations are required to characterize the performance of each evaluated technology.

5.2.2 Data and knowledge acquisition

Raw data were acquired from operational measurements and analyses performed by operators of each WWTP and were available from an internal server database. The datasets were automatically imported and adapted to the format required by the tool. Each dataset was categorized by system –i.e., by WWTP– and year and comprised 38 measures (as shown in Table 12). Hence, data input management was standardized in timestamp matrices of 38 columns and 365 rows –i.e., 1 row per day– for each WWTP included in the simulation.

Table 12. Summary of data used for WWTP simulation

ID	**Description**	**Unit**	**Frequency of measurement**
	Water Line (13 components)		
Qin	Input Flow	m3/d	365/year
BODin	Input Biodegradable Oxygen Demand	mg/L	150/year
CODin	Input Chemical Oxygen Demand	mg/L	150/year
Nin	Input Total Nitrogen	mg/L	150/year
Pin	Input Total Phosphorous	mg/L	150/year
Sin	Input Solids	mg/L	130/year
Qout	Output Flow	m3	150/year
BODout	Output Biodegradable Oxygen Demand	mg/L	150/year
CODou	Output Chemical Oxygen Demand	mg/L	150/year
Nin	Output Total Nitrogen	mg/L	150/year
Pout	Output Total Phosphorous	mg/L	150/year
Sout	Output Solids	mg/L	130/year
Tww	Wastewater temperature*	°C	320/year
	Sludge Line (18 measures)		
Qps	Primary Sludge Flow	m3/d	365/year
Sps	Primary Sludge Solids	% wet mass	100/year
VSps	Primary Sludge Volatile Solids	% dry mass	100/year
Qp	Biological Sludge Flow	m3/d	365/year
Sp	Biological Sludge Solids	% wet mass	150/year

Table 12 (continuation)

ID	Description	Unit	Frequency of measurement
VSp	Biological Sludge Volatile Solids	% dry mass	150/year
Spst	Thickened Primary Sludge Solids	% wet mass	100/year
Spt	Thickened Biological Sludge Solids	% wet mass	100/year
Qdin	Anaerobic Digestion Input Flow	m3/d	365/year
Sdin	Anaerobic Digestion Input Solids	% wet mass	100/year
VSdin	Anaerobic Digestion Input Volatile Solids	% dry mass	100/year
Sdout	Anaerobic Digestion Output Solids	% wet mass	100/year
VSdout	Anaerobic Digestion Output Volatile Solids	% dry mass	100/year
Qc	Dehydration Input Flow	m3/d	365/year
Qbt	Biogas Flow	m3/d	365/year
Kfd	Dehydrated Sludge Mass	kg/d	365/year
Sfd	Dehydrated Sludge Solids	% wet mass	50/year
VSfd	Dehydrated Sludge Volatile Solids	% dry mass	50/year
	Minor Wastes (3 measures)		
Ksand	Sand Waste Mass	kg/d	365/year
Kgreix	Grease Waste Mass	kg/d	365/year
Kdesb	Screening Waste Mass	kg/d	365/year
	Reagent Measures (2 measures)		
Kphos	Ferric Chloride Consumption	kg/d	365/year
Kpoli	Polyelectrolyte Consumption	kg/d	365/year
	Energy Balance Measures (2 measures)		
Et	Total Electricity Consumption	kWh/d	365/year
Ep	Total Electricity Production	kWh/d	365/year

Information was acquired through interviews with operators and managers related to the sanitation system under study, as well as through extensive analysis of the literature. This information was used to characterize the simulation processes related to each technology included in the simulation (both conventional and innovative technologies). Inputs, outputs and potential KPIs were identified for each simulated process (for more detail, see the “Model Implementation” section).

5.2.3 Cognitive analysis

The acquired knowledge from the previous step (“Data and knowledge acquisition stage”) was used in combination with the stated objective and requirements of the tool. A KPI hierarchy was designed by the authors, based on common drivers of the wastewater sector to decide to which level of the hierarchy assign each indicator. KPIs have been used as a means to process a wide variety of information regarding different aspects of WWTP impacts, costs and benefits for each of the potential scenarios and to characterize the performance of the most relevant functions (such as energy consumption, nutrient mass balance and process stability). The hierarchy of the KPIs was designed with three levels, namely, the top level, including five KPIs that are envisioned as helping decision-makers at a regional scale, i.e., considering the impacts of new WWTP development and planning for the sanitation system; the intermediate level, including 14 KPIs dedicated to decision-maker assessments at the WWTP level; and the lower level, with 19 KPIs that gather most of the daily information required by operators in order to properly supervise the daily performance of the WWTP and detect anomalies or abnormal tendencies. For further information about each KPI, see Table 13.

The KPIs from the top level, i.e., layer 1, are designed to agglomerate all the issues concerning the concept of sustainability. Specifically, KPI L1_1 (viability index) corresponds to the equally weighted and normalized sum of the other four KPIs in layer 1 and that attempts at condensing the most relevant KPIs regarding top-level decision making (it is assumed that all of the KPIs involved are highly relevant to guarantee project viability, so that’s the reason why they are equally weighted). The material circularity index (KPI L1_2) indicates how much material, e.g., fuels, nutrients, metals, is recovered compared to the theoretical maximum recoverable amount. The energy self-sufficiency index (KPI L1_3) quantifies the sum of all energy consumed against that it is produced by the same system, without differentiating the energy type (i.e. electrical or thermal). The risk and impacts index (KPI L1_4) is designed to condense the information from the KPIs of the lower levels, i.e., layer 2 and layer 3, and indicate how many of them show values that exceed normality. The economic assessment (KPI L1_5) describes the economic balance, basically through the calculation of the Net Present Value (NPV). Note that further amortisation beyond the correspondent technology lifespan used (10 years) hasn’t been considered. The design of the KPIs in layer 2 and layer 3 is based on commonly used performance indicators for WWTPs, as indicated in [72,73].

Table 13. KPI hierarchy. Where PE means "Population Equivalent", a measure unit that equals to 60g of biochemical oxygen demand (BOD).

ID	Description	Units
	Layer 1 (regional level)	
L1_1	Viability index	-
L1_2	Material circularity index	% of maximum recoverable
L1_3	Energy self-sufficiency index	% of total consumption
L1_4	Risk & impacts index	% of KPIs over alert threshold
L1_5	Economic assessment	NPV (M€)
	Layer 2 (plant level)	
L2_1	Organic load	PE*/m3
L2_2	Organic matter elimination	% COD
L2_3	Nitrogen elimination	% total nitrogen
L2_4	Total wastes produced	kg/d
L2_5	Total biogas produced	Nm3/d
L2_6	Anaerobic digester efficiency	% COD converted
L2_7	Total emissions produced	kg CO2 eq/d
L2_8	Energy efficiency (to total flow)	kWh/m3
L2_9	Electricity self-sufficiency	%
L2_10	Thermal balance	Thermal kW/d
L2_11	Energy circularity index	% of maximum recoverable
L2_12	Waste management cost	€/day
L2_13	OPEX (operational expenditures)	€/day
L2_14	CAPEX (capital expenditures)	€
	Layer 3 (process level)	
L3_1	Wastewater flow	m3/d
L3_2	Biodegradable organic load	%BOD/COD
L3_3	Phosphorous elimination	% total phosphorous
L3_4	Solids elimination	% solids content
L3_5	Overflow of untreated wastewater	% of flow

Table 13 (continuation)

ID	Description	Units
L3_6	Sludge production	kg/m3
L3_7	Sand production	kg/m3
L3_8	Grease production	kg/m3
L3_9	Screenings production	kg/m3
L3_10	Biogas production	Nm3/PE*·year
L3_11	Organic matter balance of anaerobic digestion	%COD input to digesters
L3_12	Electricity consumption	kWh/d
L3_13	Energy efficiency (to organic matter)	kWh/kg BOD eliminated
L3_14	Energy efficiency (to total nitrogen)	kWh/kg N eliminated
L3_15	Electricity production	kWh/d
L3_16	Electricity production efficiency	kWh/Nm3 biogas
L3_17	Phosphorous elimination efficiency	kg eliminated P/kg ferric salts
L3_18	Sludge dehydration efficiency	kg polyelectrolyte/t MS sludge
L3_19	Reagent consumption cost	€/d

5.2.4 Model selection

The methodology presented here is based on a simulation model (with KPIs as outputs). Each scenario corresponds to a WWTP and its corresponding dataset with a specific technology configuration (either the current configuration or another that includes new processes). The simulation model comprises mass, nutrient and energy balances for each process of the sewage sludge line (similarly as in [34,56]), raw emissions estimates and economic assessments (for the latter, NPV was calculated assuming a 4% discount rate and a lifespan period of 10 years). Performance parameters are required to properly simulate some processes and were estimated from existing data or theoretical estimations. The raw input to this simulation method consists of the different physical, chemical and energetic inputs and outputs of each process. The KPIs were computed from this raw input and other input data, e.g., stoichiometric and process parameters and economic pricing of commodities and disposal costs (which are determined for each case study, and whose values used for the present study can be seen at the "Case study" section).

5.2.5 Model implementation

The model presented here was implemented in a software tool developed in MATLAB-SIMULINK. MATLAB is a widely used numerical computing and programming platform at many research institutions and organisations, which makes it a convenient prototyping and development framework. SIMULINK is a visual programming environment that allows the integration of MATLAB code; this suits the purpose of the tool presented here, which aims to develop a set of toolboxes for each of the processes considered in its development. Hence, the simulation model was integrated into the SIMULINK environment, a visual programming environment in which each process considered was implemented as a system block (i.e., a self-contained unit of code related to at least one process of the system). A tailored process library was created with these process building blocks.

The aim of the DSS-WWTP simulator tool is to provide an assessment for different combinations of existing or potential technologies by simulating each scenario and assessing the performance of the WWTP with the KPIs. Thus, the use of a library for the different implemented technologies and the KPIs as the output of the simulation for assessment is a core feature of the presented tool. Overall, the developed DSS-WWTP simulator has two main modules: the process library and the WWTP simulator. The WWTP simulator module includes two submodules, namely, the process simulation and the KPI calculation. The scheme of the presented tool and its modules is summarized in Figure 12.

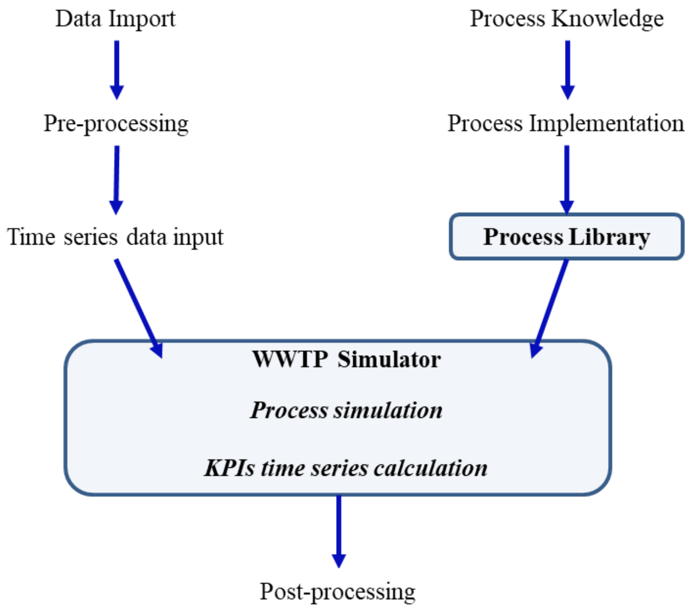

Figure 12. Scheme of the developed DSS-WWTP simulator tool. The two main modules (Process Library and WWTP Simulator) are highlighted.

The data import phase involves the extraction of raw data (in a daily time-series format) from WWTP practitioner databases. The pre-processing phase involves data conditioning techniques to adapt gathered data to the format required by the MATLAB platform (the time-series data input format) such as integration, sorting and validation. On the other hand, process knowledge refers to the collection of information related to the performance of and the"basic concepts regarding each of the processes involved in the simulated system (i.e., the processes involved in a WWTP).

The process library includes each WWTP process that is implemented in the simulation tool, as in the following procedure: first, identification, definition and classification of all unit operations of the WWTP are performed, as well as a qualitatively determination of the corresponding key added value of each unit to the overall performance, according to conventional standards as those described in [72,73]. Second, a set of technological options are determined for each unit operation (including the no-implementation alternative for the corresponding operation unit). Then, for each technological option (of each unit operation), the process inputs and outputs are determined. Finally, for each process input and output, the minimum significant parameters are identified, as well as whether they are available for each WWTP to be simulated; if they are not available, their computation by estimation, stoichiometry, mass balance assumptions or other mathematical approaches is considered (taking into account that parameters with relatively high variability or time-dependent deviations will be measured and not assumed as constant values).

The current version of the developed tool presented here consists of four unit operations. Each of these four unit operations considers one of their most representative technologies (the ones already implemented at full scale and well known across the wastewater sector) and, by default, they also consider their absence. That way, simulations can be done with different configurations of technologies (i.e. different WWTP process layouts) resulting from the combination of each one of these technologies and also enables the possibility of neglecting the use of one or more of these unit operations to design the scenarios.

The four unit operations of the tool under study are sludge conditioning, sludge drying, sludge thermal valorisation and biogas valorisation. The first three unit operations have one technology implemented: thermal hydrolysis (TH), conventional sludge drying (SD) and thermal valorisation (TV), respectively. These selected technologies are representative of each of their corresponding unit operations, and the possibility to neglect the use of these technologies is included. For example, each scenario can consider TH or not, in which case it is represented as NP (No Pretreatment) instead of TH; for the cases of SD and TV, their correspondent counterparts that reflect the absence of such technology are noted as ND and NTV, respectively.

Biogas valorisation involves two different technologies: biogas cogeneration (BC) and biogas upgrading (BU), but the possibility of neglecting biogas valorisation (i.e. including in the simulation a "no biogas valorisation") is not considered. The implementation procedures for each of the aforementioned technology options (i.e., TH, SD, TV, BC and BU) are shown in Table 14, Table 15, Table 16, Table 17 and Table 18, respectively. Note that anaerobic digestion (if present, which is the case of the case study) is modelled according to the data from each case study (as shown in Table 12).

Table 14. Process implementation for thermal hydrolysis

Process implementation procedure	Example of application to thermal hydrolysis
Unit Operation	Thermal Hydrolysis
Added value to WWTP	Reduction in the volume of sludge and hygienization Increase in biogas production
Technological options	Thermal Hydrolysis (TH)
Process inputs:	Thickened Sludge & Thermal Energy
Significant input parameters	Mass, Dryness & Thermal Energy demand
Mass estimation	Measured in plant
Dryness estimation	Measured in plant
TE demand estimation	Assumption from the average performance of TH
Process outputs:	Hydrolysed Sludge
Significant output parameters	Mass & Dryness
Mass estimation	Calculation by mass balance of inputs and outputs
Dryness estimation	Calculation by mass balance of inputs and outputs

Table 15. Process implementation for sludge drying

Process implementation procedure	**Example of application to sludge drying process**
Unit Operation	Sludge Drying
Added value to WWTP	Reduction in the volume of sludge and hygienization
Technological options	Conventional Sludge Drying (SD)
Process inputs:	Dehydrated Sludge & Thermal Energy
Significant input parameters	Mass, Dryness & Thermal Energy demand
Mass estimation	Measured in plant
Dryness estimation	Measured in plant
TE demand estimation	Assumption from average performance of the SD
Process outputs:	Dry Sludge
Significant output parameters	Mass & Dryness
Mass estimation	Calculation by mass balance of inputs and outputs
Dryness estimation	Assigned as design parameter: set at fixed value

Table 16. Process implementation for thermal valorisation

Process implementation procedure	**Example of application to thermal valorisation**
Unit Operation	Thermal Valorisation
Added value to WWTP	Reduction in the volume of sludge produced as ashes Energy generation
Technological options	Conventional Thermal Valorisation (TV)
Process inputs:	Dry Sludge & Thermal Energy
Significant input parameters	Mass, Calorific Value & Ashes
Mass estimation	Measured in plant
Calorific Value estimation	Measured in laboratory
Ashes estimation	Measured in laboratory
Process outputs:	Ashes, Emissions & Energy Balance
Significant output parameters	Ash Mass, Emissions & Energy Balance
Ash Mass estimation	Calculation by mass balance of inputs and outputs
Emissions estimation	Assumption from average performance of the TV
Energy Balance estimation	Assumption from average performance of the TV

Table 17. Process implementation for biogas cogeneration

Process implementation procedure	**Example of application to biogas cogeneration**
Unit Operation	Biogas Valorisation
Added value to WWTP	Processes biogas to generate a product
Technological options	Biogas Cogeneration (BC)
Process inputs:	Biogas
Significant input parameters	Mass & Methane
Mass estimation	Measured in plant
Methane estimation	Measured in laboratory
Process outputs:	Electrical Energy, Thermal Energy, Emissions
Significant output parameters	Electrical Energy, Thermal Energy & Emissions
EE estimation	Assumption from average performance of the BC
TE estimation	Assumption from average performance of the BC
Emissions estimation	Assumption from average performance of the BC

Table 18. Process implementation for biogas upgrading

Process implementation procedure	**Example of application to biogas upgrading**
Unit Operation	Biogas Valorisation
Added value to WWTP	Processes biogas to generate a product
Technological options	Biogas Upgrading (BU)
Process inputs:	Biogas
Significant input parameters	Mass & Methane
Mass estimation	Measured in plant
Dryness estimation	Measured in plant
Process outputs:	Biomethane
Significant output parameters	Mass & Emissions
Mass estimation	Calculation by mass balance of inputs and outputs
Emissions estimation	Assumption from average performance of the BU

The WWTP simulation module consists of a basic WWTP simulation scheme containing selected processes drawn from the process library. A scenario is created once the data inputs and the WWTP configuration (generated by combining the WWTP simulation scheme with the selected library processes) are established. Therefore, for a WWTP, each scenario consists of its corresponding data set (shown in Table 12) and the overall configuration of the building blocks of the simulation scheme created from the basic blocks and the processes selected from the process library.

The KPIs are calculated and ordered as shown in Table 13 for each of the simulated scenarios based on the different parameters of the simulation (the inputs and outputs of several of the processes involved). Validation tests of this tool were carried out with a real WWTP as a case study.

5.3 Results

5.3.1 Case study

The proposed tool was tested with a case study WWTP of a real sanitation system comprised within Consorci Besòs Tordera (CBT) environment. CBT is a public local water administration composed of 64 municipalities in four different regions of Catalonia (Spain) with a population of approximately 470,000 inhabitants that manages 26 sanitation systems. The area served by these WWTPs features a contrast between high anthropic-pressure areas (urban and industrial, relatively close to the metropolitan area of Barcelona) and other rural areas.

The WWTPs managed by CBT have a treatment capacity ranging from 1,000 to 30,000 m3/d, and they are located in the northern region of Barcelona, specifically in the upper parts of the Besòs River basin and the Tordera River basin. Figure 13 shows a map of the WWTPs of the sanitation system. Specifically, in this work, the DSS-WWTP simulator tool was tested in the Granollers municipality’s WWTP (GR WWTP), which is one of the most representative WWTPs from the 26 sanitation systems of CBT due to its treatment capacity and the high anthropogenic impact of its wastewater.

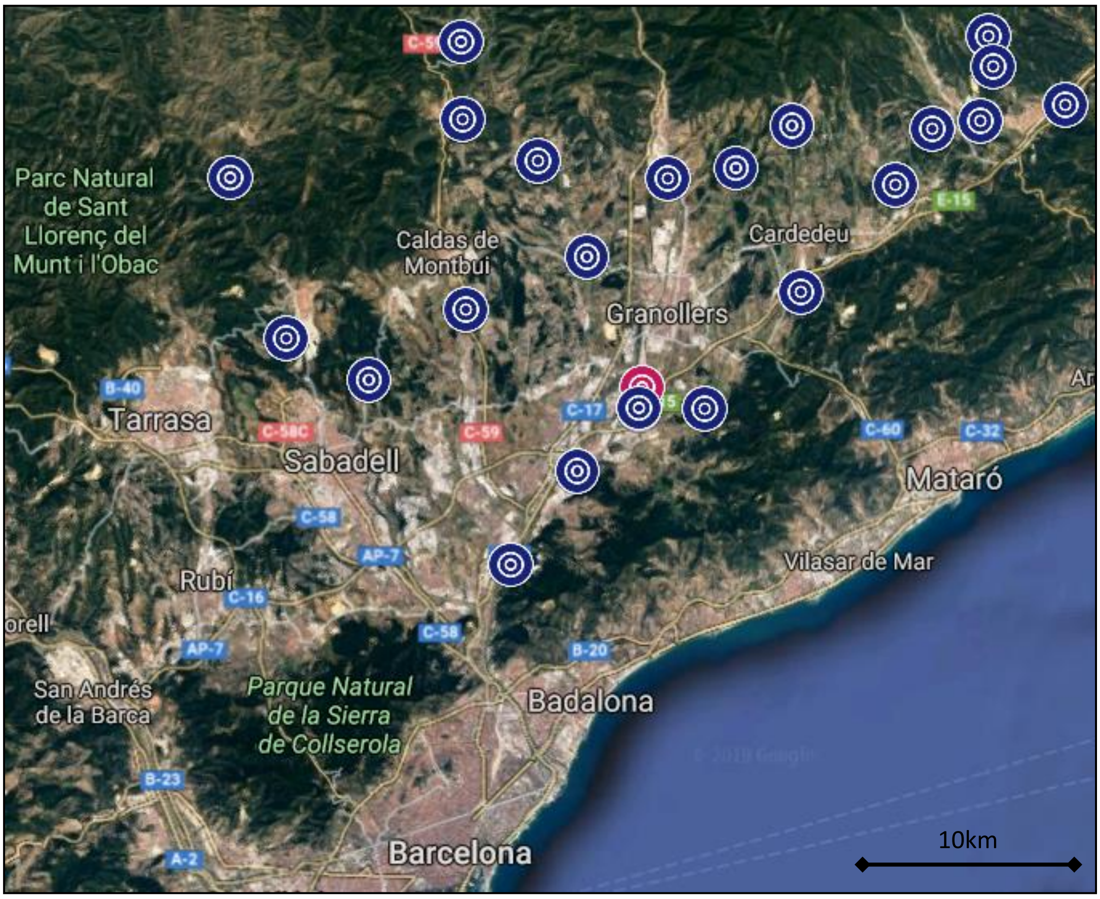

Figure 13. Map of the wastewater treatment system under study, where each dot corresponds to a WWTP. GR WWTP corresponds to the red dotted WWTP.

Eight scenarios were simulated for the GR WWTP, created by combining the unit operation technologies shown in Table 14-Table 18. Table 19 lists each scenario and its corresponding configuration. Note that thermal valorisation (TV) is always considered together with sludge drying (SD) because the latter is a required process before enabling sludge thermal valorisation; on the contrary, sludge drying is not considered without thermal valorisation in this case study.

Table 19. Scenarios and corresponding process configuration for the GR WWTP case study. Where NP is "no pretreatment", TH is "thermal hydrolysis", ND is "no sludge drying", SD is "sludge drying", NTV is "no thermal valorisation", TV is "thermal valorisation", BC is "biogas cogeneration" and BU is "biogas upgrading".

	Scenarios							
Unit operations	1	2	3	4	5	6	7	8
Sludge conditioning	NP	NP	NP	NP	TH	TH	TH	TH
Sludge drying	ND	SD	ND	SD	ND	SD	ND	SD
Sludge thermal valorisation	NTV	TV	NTV	TV	NTV	TV	NTV	TV
Biogas valorisation	BC	BC	BU	BU	BC	BC	BU	BU

To perform economic analysis, NPV (i.e. KPI L1_5) has been calculated for scenarios 2-8. Their correspondent cash flows already accounts for savings expected in comparison to scenario 1 cash flow (the current plant layout). Based on data gathered from interviews with expert consultants of the processes involved, an investment cost was approximated to each technology: 4,000,000 € for both thermal valorisation and sludge drying process (TV and SD, which will be considered simultaneously in this case study, as shown in scenarios 2, 4, 7 and 8), 5,000,000 € for biogas upgrading technologies, and 3,000,000 € for thermal hydrolysis technologies. In addition, to complete the cost-benefit analysis, costs were assigned to each different waste generated according to cost trends of the last years in Catalonia: for dehydrated sludge, 50 €/ton; for ashes (obtained after sludge thermal valorisation), 80 €/ton; and for other minor wastes (such as those from the pre-treatment of the water line), 80 €/ton. Additionally, an electricity price of 0.1005 €/kWh was assigned for electricity consumption of the case study. To perform the economic assessment (i.e., KPI L1_5) the NPV was calculated using the aforementioned data, assuming a discount rate of 4% and a time period of 10 years. Also, note that inversion costs considered to calculate the NPV are related only to technology acquisition and installation, without further including additional costs related to required adaptations of the WWTP to the new technologies.

5.3.2 Scenario comparison

The application of the DSS-WWTP simulator tool to the eight scenarios in the case study of the representative GR WWTP in the CBT environment allowed the integrated assessment of each of the technologies involved in the simulation via pair-wise comparison. Scenario 1 includes the technologies corresponding to the current configuration of the real GR WWTP (that is, the control scenario). Note that since scenario 1 does not include any investment cost, its NPV is not expressed when calculating KPI L1_5. The results are shown as annual averages with their corresponding deviations. However, the presented tool also allows us to show KPIs as a time series, as shown in Figure 14. For the sake of brevity, in this work, an array of six representative KPIs was selected from the full list to simplify data analysis and discussion, as shown in Figure 15.

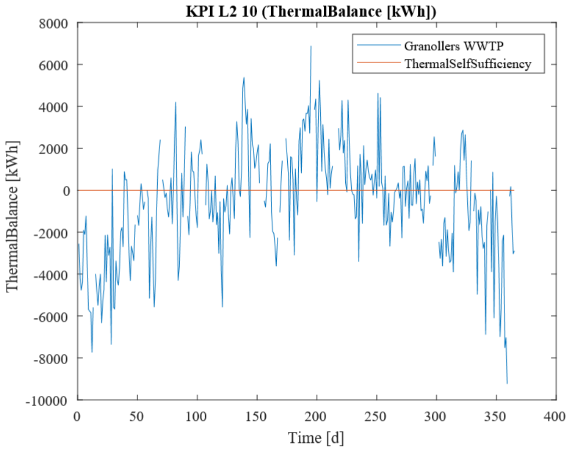

Figure 14. Sample time-series graph of KPI L2_10 (Thermal Balance) for scenario 1.

The results in Figure 15 show that there are large deviations (accounting for 20-50% of most KPIs) compared to the standard tolerance margin of 10% deviation that is applied for real plant measurements. This is probably because average annual data were used. It is important to highlight that KPI L2_10 (thermal balance) shows different deviations in each scenario, since it is strongly affected by the temperature and, thus, by seasonal variations within the corresponding year. Annex shows KPI L1_5 for each scenario with further detail.

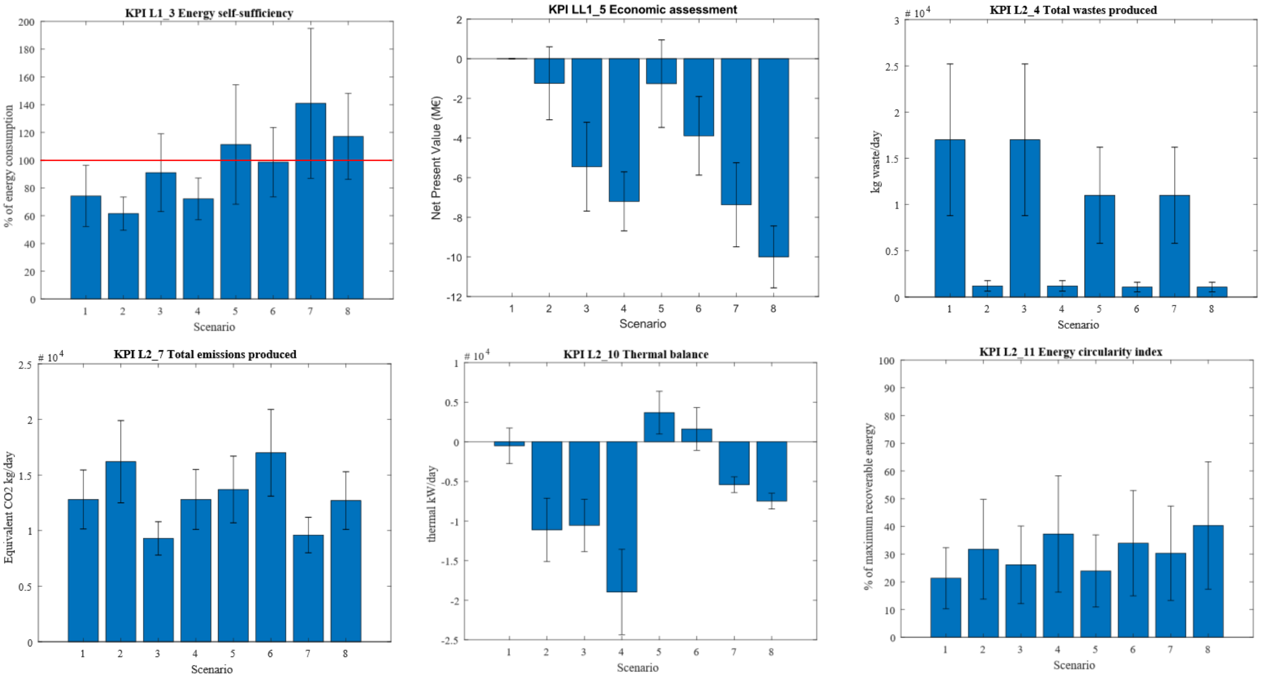

Figure 15. Annual averages and standard deviations for six KPIs from the simulation of the annual dataset of the GR WWTP applied to eight scenarios.

Only scenario 7 seems to be clearly energy-positive, since KPI L1_3 indicates that the energy produced exceeds 100% of the energy consumed; Scenario 5 would also seem energy positive, but their associated variabilities are significantly high, reaching a minimum of 70% energy self-sufficiency. Besides, note that this KPI refers to both electricity and heat balances. The economic balance (i.e., KPI L1_5) indicates that scenarios 2 and 5 have the best NPV results (about -1.2 M€ each).

As shown by KPI L2_4, waste production was drastically reduced in scenarios with thermal valorisation (that is, scenarios 2, 4, 6 and 8, where a reduction of approximately 90% was achieved). Scenarios 5 and 7 also allow waste production reductions of up to approximately 30%. The trend observed for total CO2 equivalent emissions (KPI L2_7) seems to favour scenarios 3 and 7 (which show 30% lower emissions than scenario 1) and penalize scenario 6 (with an emissions increase of approximately 30% compared with that in scenario 1).

KPI L2_10 may be interpreted as the overall average thermal balance over a year. Thus, its deviations can be interpreted as the upper and lower ranges of thermal balance for the hottest and coldest seasons of the year, respectively. Scenario 1 shows a thermal balance around thermal equilibrium (the zero mark), with a lower deviation range dipping into the negative zone (up to approximately -2,500 kW/day). This indicates that during the coldest seasons of the year, the current GR WWTP (as its current technology is represented in scenario 1) might have a thermal demand of approximately 2.5 MWh/day. Only scenarios 5 and 6 show a positive thermal balance (thus having excess thermal production). Scenarios 2, 3, 4, 7 and 8 clearly show negative thermal energy balances, accounting for 11,100, 10,600, 19,000, 5,400 and 7,500 kW/day for each scenario, respectively.

Finally, KPI L2_11 shows how much energy may be recovered by the plant itself compared with the maximum theoretical thermodynamic energy recoverable from the organic matter input to the plant. As a general trend, scenarios 1 and 5 show the lowest energy recovery ratios (approximately 22%), while those scenarios with sludge thermal valorisation (i.e., scenarios 2, 4, 6 and 8) allow around a 50% more energy recovery (around 30-35%% total energy recovery). The average energy recovery for scenarios 3 and 7 is in between these values (around 25-30%). However, note that for this specific KPI, all scenarios have deviations of approximately 50% of the average value. Thus, only qualitative comparisons are viable.

5.3.3 Technology comparison

The potential impacts of each technology in the selected KPIs are determined in this section with a pair comparison strategy. Since each scenario is affected by a combination of multiple technologies, each with their own effects on the KPIs, the pair-wise comparison allows us to discern the effects of each technology. However, KPI L2_10 is not included in the tables in this section because its values are discussed based on the minimum and maximum values attained for thermal balances as shown in Figure 15. Also, note that NPV of scenario 1 is not accounted because it doesn't involve any inversion costs (instead, the annual cash flow used to calculate the NPV of the other scenarios corresponds to the differential with that of scenario 1).

Table 20 summarizes the results for each pair of scenarios with and without thermal valorisation. The scenarios with thermal sludge valorisation (i.e., scenarios 2, 4, 6 and 8) show (compared with their counterparts, i.e., scenarios 1, 3, 5 and 7, respectively) a decrease in energy self-sufficiency (KPI L1_3) ranging from -10% to -25%; a decrease between 35% and 200% in the NPV value (KPI L1_5) is achieved (i.e. higher costs); a decrease of 90% in waste production (KPI L2_4); an increase in emissions (KPI L2_7) ranging from 25% to 35%; and an increase in the total energy recovered ranging from 40% to 50% (KPI L2_11). For the thermal balance (KPI L2_10), for scenario pairs 1-2 and 3-4, there is an increase in demand of 10,600 kW/day and 8,400 kW/day, respectively; on the other hand, for both scenario pairs 5-6 and 7-8, the thermal demand increases by 2100 kW/day for each of those pairs.

Table 20. Comparison of scenarios based on thermal valorisation technology analysis.

KPIs	**Scenarios compared**			
	1 -2	3-4	5-6	7-8
L1_3	-15%	-20%	-10%	-15%
L1_5	-	-30%	-200%	-35%
L2_4	-90%	-90%	-90%	-90%
L2_7	30%	35%	25%	30%
L2_11	50%	40%	40%	30%

Table 21 summarizes the results for each pair of scenarios with and without biogas upgrading. The scenarios with biogas upgrading technologies (i.e., scenarios 3, 4, 7 and 8) show (compared with their counterparts, i.e., scenarios 1, 2, 5 and 6, respectively) an increase in energy self-sufficiency (KPI L1_3) ranging from 15% to 30%; a decrease of NPV (KPI L1_5) ranging around 160% to 480% (i.e. higher costs); no change in waste production (KPI L2_4); a decrease in emissions (KPI L2_7) ranging from 25% to 30%; and an increase in the total energy recovered ranging from 15% to 30% (KPI L2_11). For the thermal balance (KPI L2_10), for scenario pairs 1-3 and 2-4, there is an increase in demand of 10,000 kW/day and 7,800 kW/day, respectively; however, for both scenario pairs 5-7 and 6-8, the thermal demand increases by 9,100 kW/day.

Table 21. Comparison of scenarios based on biogas upgrading technology analysis

KPIs	**Scenarios compared**			
	1-3	2-4	5-7	6-8
L1_3	20%	15%	30%	20%
L1_5	-	-480%	-480%	-160%
L2_4	0%	0%	0%	0%
L2_7	-25%	-25%	-30%	-25%
L2_11	25%	15%	30%	20%

Table 22 summarizes the results for each pair of scenarios with and without thermal hydrolysis. The scenarios with thermal hydrolysis (i.e., scenarios 5, 6, 7 and 8) show (compared with their counterparts, i.e., scenarios 1, 2, 3 and 4, respectively) an increase in energy self-sufficiency (KPI L1_3) ranging from 50% to 60%; a decrease of NPV (KPI L1_5) ranging around 35% to 210% (i.e. higher costs); a decrease between 10% to 35% in waste production (KPI L2_4); an increase in emissions (KPI L2_7) ranging from 0% to 15%; and an increase in total energy recovered ranging from 5% to 15% (KPI L2_11). Regarding the thermal balance (KPI L2_10), for scenario pairs 1-5 and 3-7, there is a decrease in demand of 4,200 kW/day and 5,100 kW/day, respectively; however, for scenario pairs 2-6 and 4-8, the thermal demand decreases by 12,500 and 11,300 kW/day, respectively.

Table 22. Comparison of scenarios based on thermal hydrolysis technology analysis

KPIs	**Scenarios compared**			
	1-5	2-6	3-7	4-8
L1_3	50%	60%	60%	60%
L1_5	-	-210%	-35%	-40%
L2_4	-35%	-10%	-35%	-10%
L2_7	10%	0%	0%	0%
L2_11	15%	5%	15%	10%

5.4 Discussion

The presented tool has the purpose of performing holistic scenario analysis by considering the impacts, costs and benefits of the implementation of new processes by means of KPI analysis. In addition, the hierarchical organisation of the KPIs in three decision-making layers or levels is meant to provide rapid scenario analysis based on to the priorities of the decision-maker. For example, if the implementation of a new process should be more focused on, e.g., the technical and performance aspects of critical WWTP functionalities, then the KPIs in layer 2 and layer 3, i.e., the plant and process levels of decision-making, respectively, should be given more importance when drawing conclusions).

The use of daily measurements as input data and the nature of the implementation of the simulation model allow a daily timeline of each KPI to be obtained for each scenario, as shown for the KPI L2_10 in Figure 14. This feature enables further time-dependent (e.g., seasonal) analysis. However, in this work, major trends based on overall yearly data were determined for the real case study to simplify data analysis and discussion.

It is important to highlight that further combinations of these scenarios can be performed and are important for identifying the appropriate implementation combination for the processes according to the criteria applied for each case study. One of the main motivations to develop the presented tool revolves around circular economy, with a special focus on the optimisation of waste management strategies and the sludge line of WWTPs to improve their overall performance. Hence, the tool provides value and applicability for decision support in real facilities.

Scenarios with thermal hydrolysis (i.e., scenarios 5, 6, 7 and 8, respectively) might allow WWTPs to increase their current percentage of energy self-sufficiency by a relative 50-60% (note that it is a relative increase in relation to the original percentage of this KPI, instead of an absolute percentage point increase), allowing, for the case of scenario 8, to reach a seemingly energy-positive WWTP. If the most energy-positive WWTP with minimal economic costs is desired, scenario 5 would be the most suitable (although it presents an NPV of -1.2M€ and its energy self-sufficiency has significant variability). Hence, the implementation of thermal hydrolysis before anaerobic digesters and thermal valorisation (the layout implemented in the WWTP simulation model) would be the best studied setup for achieving a potentially energy-positive WWTP according to the method presented.

As a general trend, thermal valorisation scenarios (i.e., scenarios 2, 4, 6 and 8) present major benefits in terms of waste reduction but also present the highest emissions increases (by 25 to 35%), with some of the most demanding thermal energy balances. However, they also present the highest values of the energy circularity index (KPI L2_11) since thermal valorisation allows major energy recovery from sewage sludge's organic matter. Despite the remarkable energy recovery achieved in these scenarios, higher amounts of energy are also required to sustain the whole process (especially due to heat demand to dry sludge before its thermal valorisation). Yet, combined thermal valorisation of sewage sludge with other external organic fuels (such as those from green biomass) might enhance the energy balance of the thermal valorisation process (a strategy that hasn't been addressed in this work).

It is important to highlight that thermal hydrolysis combined with thermal valorisation (scenarios 6 and 8) presents a synergy from an energy optimisation perspective (since it reduces the need for thermal energy demand, thus increasing energy self-sufficiency when compared to scenarios 2 and 4, respectively). Actually, thermal hydrolysis seems to neglect the reduce the thermal energy demand from implementation of thermal valorisation when comparing scenario pairs 5-6 and 7-8 (where thermal balance demand just increases by about 2,100kW while for the analogous thermal valorisation implementation scenario pairs 1-2 and 3-4 thermal demand increases by 10,600 and 8,400 kW, respectively). Hence, if energy recovery maximisation is a priority, scenarios 7 and 8 would be the most applicable, but they would come at a significant cost (with NPV values around -7.4 and -10.0 M€, respectively).

On the other hand, biogas upgrading is a well-known process that has been studied in many recent works due to its better performance than co-generation in biogas valorisation; see, e.g., [35,74]. The efficiency of this process is shown in scenario 3: it allows an increase in the energy recovery of 15-30% and an emissions reduction of 25-30%. However, the economic cost increases considerably (NPV for biogas upgrading technology is estimated around -5.5M€, as shown for scenario 3), and the replacement of the conventional co-generation biogas valorisation in the upgrading process (where it is assumed that upgraded biogas is injected to the grid and is thus not available for heat generation) reduces the heat available from co-generation. Thus, scenario 3 has a thermal demand of approximately 10,600 kW/day, and scenario 4 has an even higher thermal demand (19,000 kW/day). Their counterpart scenarios with thermal hydrolysis (i.e., scenarios 7 and 8) show remarkably lower thermal energy demands (approximately 5,400 and 7,500 kW/day, respectively) but with an increase in economic costs (i.e. NPV) about 40% (the highest among all scenarios studied, as observed with comparing scenario pairs 3-7 and 4-8). Hence, thermal hydrolysis presents this additional synergy with biogas upgrading (in terms of thermal balance) but at the expense of having the highest economic costs among all the scenarios considered. Although biogas upgrading does not currently provide significant improvements to WWTP performance if its economic cost is taken into account, its true feasibility depends on the evolution of national energy markets, and it may become more beneficial in the future.

Thus, if the practitioner is looking for a sustainable transition from scenario 1 with a minimal economic cost increase, scenario 5 would be the most economically feasible (with an NPV of -1.2M€). It has no significant impact on emissions increase (nor decrease) while guaranteeing a positive thermal balance and an overall energy-positive WWTP, as shown by KPI L1_3. Besides, it is important to note that in a sector which provides essential public services such as wastewater treatment, projects with negative NPV doesn’t strictly imply unviability of such project. Furthermore, thermal hydrolysis allows synergies (related to the thermal balances) with both thermal valorisation and biogas upgrading technologies; for instance, it seems that thermal valorisation would not add an increase of thermal demand if it is implemented after thermal hydrolysis.

To face the upcoming challenges for sewage sludge valorisation in the context of the circular economy, practitioners are looking for a holistic waste management strategy, i.e., a strategy that considers the whole set of available sanitation facilities and their features. Thus, if environmental criteria are prioritized, scenarios 3 and 7 would be the most beneficial among the scenarios considered here to allow the circular economy transition, both based on the implementation of biogas upgrading (allowing about 25-30% emission decrease) but at higher costs (around NPV of -5.5M€ and -7.4M€, respectively). On the other hand, if economic criteria are prioritized, scenario 5 would be the most feasible (revolving around thermal hydrolysis, or waste-to-energy); although both scenario 5 and scenario 2 presents almost the same NPV value, scenario 5 (thermal hydrolysis) shows additional benefits (such as guaranteeing a positive thermal balance with further related synergies to implementation of other technologies, no emission increase and a still significant waste reduction).

Finally, the existence of different DSS-optimisation methods that allow us to avoid exhaustive manual analyses of different combinations of technologies and propose an optimal solution according to certain optimisation criteria should be mentioned; see, e.g., [29,37,45,67,75–77]. The tool presented here is not focused on this feature; however, its simulation-based nature and its design will allow the implementation of such optimisation techniques in future stages, providing an automated optimal outcome for the design process. The proposed tool aims to be a support tool for practitioners that provides sanitation system simulation and analysis in order to perform a rapid and holistic analysis of system performance and hence to enable potential enhancements to operational decision-making, as shown here in the considered case study.

5.5 Conclusions

The presented DSS-WWTP simulator tool is based on a combination of methods (process simulation, hierarchical KPIs and scenario analysis) that are usually considered separately. The visual programming approach presented here by means of the MATLAB-SIMULINK environment allows a more intuitive design approach than other methods, with easier and more standardized implementation of the different processes. This approach also allows better reusability and scalability for the processes implemented, which are compiled in a toolbox that may be expanded with additional processes of interest for further assessment. Thus, one of the main features of the tool presented here is its ready scalability and configurability for the systems under study. The current implemented processes are related to the WWTP sludge line, since circular economy concerns related to WWTPs are mainly related to sewage sludge-related issues. However, due to the aforementioned scalability, further toolboxes for this tool may include different operational units and processes in addition to those related to the sludge line.

The case study of the GR WWTP showed that: thermal hydrolysis is the most suitable technology considering the aforementioned estimations and assumptions for scenario simulation (based on mixed economic, environmental and energetic criteria) and presents synergies with the thermal balances of other technologies, such as thermal valorisation or the transition from biogas co-generation to biogas upgrading; thermal valorisation is better than thermal hydrolysis from an overall energy recovery performance, but it is less environmentally friendly and does not provide a positive thermal balance.; finally, biogas upgrading is the most expensive technology evaluated herein but allows the highest emissions reduction.

In addition, this tool could be applied as a supporting tool for asset management purposes and for long-term performance monitoring. Hence, further work may be focused on, e.g., the implementation of fault detection and isolation methods to detect and isolate abnormal behaviour involving WWTP systems. Future work will also consider the inclusion of further processes of interest in the tool process library and the optimisation of their combination to provide an optimal outcome for decision making support.

Chapter Six

Optimised blending for anaerobic co-digestion using ant colony approach: Besòs river basin case study

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6.1 Introduction

The anaerobic digestion process in WWTPs plays an important role amongst potential circular economy technologies since it is one of the most well-established and promising processes in these installations, as stated by [12,19,78]. Furthermore, the co-digestion of sewage sludge and organic wastes has arisen as a promising strategy in the circular economy due to its capability of merging both wastewater and waste valorisation value chains. However, further work is required to fully achieve the optimisation and improvement of the anaerobic co-digestion process [41,79,80]. To this end, a remarkable number of anaerobic digestion optimisation tools have been recently developed, as reported by [60]. These tools are focused on the modelling and control of the optimum co-substrate blend and operation, as shown in ([81], [82], [83], [84], [85]). For example, [81] and [83] focused on the identification and modelling of critical parameters for co-digestion, such as volatile fatty acid production and particle size, and concluded that co-digestion is highly feasible; [82] developed control schemes for anaerobic digesters based on the composition qualities; and [84] and [85] implemented optimised control strategies according to the blend composition parameters, such as the organic and nitrogen content and the inhibition thresholds of the anaerobic digestion processes (which have been identified by previous biochemical modelling efforts [17,36,86]).

However, to the best knowledge of the authors, the complex logistics—and their related economics—associated with both co-substrates and sewage sludge have not been assessed mainly due to the ad hoc nature of each study case and the lack of data in the literature from the organic waste transportation sector. In addition, there are underlying critical factors for co-substrate selection not only at the characterisation-related level but also with respect to the associated logistics. Some undesired impacts of non-optimised transportation routes of co-substrates are as follows: increases in route length, time, costs and emitted greenhouse gases (GHG); increases in traffic density (which can be an issue for highly populated and busy areas); and additional odours, noise and air pollution in urban areas (which is a major issue for pedestrian and recreational zones, such as parks and the main streets of urban areas). Logistics optimisation may provide a useful approach to tackle and avoid the aforementioned social, environmental and economic impacts.

Regarding the optimisation method, combinatorial optimisation problems such as the one presented here can be solved using the ACO algorithm ([87],[88]). ACO is a metaheuristic approach that has been shown to be effective in solving a variety of NP-hard combinatorial optimisation problems [48], such as the well-known travelling salesman problem (TSP). The

ACO algorithm searches for a solution using a probabilistic and iterative procedure that emulates the behaviour of a real colony of ants in their search for food (pheromone trails are used and updated in the algorithm). Further methods may be applied to tackle NP-hard problems, e.g., genetic algorithms (GA). GA is a metaheuristic based on the mechanics of natural selection and natural genetics; GA has also become an important tool in combinatorial optimisation problems and has been used to solve different problems of combinatorial optimisation, e.g., hydraulic model calibration [89] and sensor placement for leak detection in water distribution networks [90]. In [91], the relation between GAs and ACO is noted. Some drawbacks of GAs are noted in [89]; e.g., achieving a global optimum for large and complex systems is not guaranteed, which is also a drawback for ACO. However, the ACO algorithm uses strategies to avoid rapid stagnation of the solution in the search space of solutions. A successful approach to ACO implementation is the max-min ant system [49], which consists of limiting the pheromone trails τ within the range $[\tau_{\min}, \tau_{\max}]$. As observed above, the ACO approach was originally applied to solve the TSP, outperforming other nature-inspired algorithms, e.g., GAs [49]. In [92], it is noted how ACO is successfully applied not only to different NP-hard academic combinatorial optimisation problems but also to some real-world problems of the same kind as the one presented here, e.g., in [93], to optimise the truck routes of a gasoline distribution company in Switzerland. ACO can also be conveniently used to solve the multidimensional knapsack problem, as introduced in [94]. In the context of the current problem, the search space of solutions is represented by a bipartite graph. The set of nodes is the sludge generators and their possible volumetric contributions, and the edges are the connections between each generator and its feasible contributions of sludge. Overall, ACO is an EA that can be complemented by local optimisation, with similar drawbacks to other evolutionary algorithms as explained previously and pointed out in [89]. The max-min approximation and the use of strategies to avoid rapid stagnation of the solution in the search space have both been applied for the ACO algorithm to enhance its features and minimise the drawbacks of the use of an evolutionary algorithm.

Moreover, applications of such an enhanced algorithm have already been made for real-world cases of the waste sector ([47,94]). The optimisation problem presented in this publication is inspired by prior optimisation problems approached by the ACO algorithm: here, it not only is applied to optimise co-digestion strategies but also takes into account the potential impact of the logistics associated with the transportation route of each co-substrate. The additional features increase the problem complexity (due to the increase in variables considered by the combinatorial optimisation), so the cost function is reformulated according to the problem stated. Achieving a single global optimum with this problem is not possible. Thus, the cost function is not a convex function, and the number of local optimums is increased by the increase in complexity. The framework presented here is an approach for assessing real conditions based on a previous work [47], which focused on synthetic results. Here, the co-substrate details are obtained by considering real data from an actual sanitation network in the area of the Besòs river basin in Catalonia.

The application of the ACO algorithm allows optimisation of codigestion strategies, enhancing biogas production and minimising associated risks to the anaerobic digestion operation (e.g., overdosing and acidification); furthermore, the novel implementation of the logistics in the algorithm allows more accurate selection of co-substrates in a real substrate multi-source/multi-receptor case study, allowing cost and impact minimisation whilst maximising biogas production with the optimal set of resources, e.g., by taking into account the impacts derived from the derived logistic routes. This is achieved in this work by a novel strategy based on the simultaneous optimisation of both the substrate composition and characterisation of their transport routes provided by the ACO algorithm. The novel application for codigestion strategies considering the logistics and volume distribution may contribute to the state-of-the-art of existent anaerobic codigestion tools as shown in [60,81–85] that have been explained previously, which were more focused on the optimisation of blending and the anaerobic digestion process.

The objective of this work was to develop a new co-digestion optimisation tool based on an enhanced version of the ACO algorithm that improves the constructed solution and avoids its rapid stagnation using two local search heuristics. The optimisation problem includes both substrate biochemical characterisation (for biogas production maximisation) and logistics characterisation (for route optimisation). The effect of centralized anaerobic co-digestion is evaluated from both technical and economic perspectives. This method is applied in a real case study composed of 16 different WWTPs—4 of which include anaerobic digesters—that are managed by Consorci Besòs Tordera (CBT), a local water authority in charge of these facilities.

6.2 Materials and methods

The problem statement considers a set of substrate generators $\mathrm{w} \in \{1, \ldots, \mathrm{N}\}$. The N different substrate generators are located different distances ($\mathrm{d_w}$) from a single anaerobic digester (ST). Each generator has the capacity to store its own substrate until it is transported to the ST. Each substrate is characterised by its volume $\mathrm{V_w}$ and a set of values $\mathrm{C_w^c}$, where $\mathrm{C_w^1}$ is the chemical oxygen demand (COD) concentration, C_w^2 is the ratio of chemical oxygen demand and total nitrogen (COD/TN), C_w^3 is the alkalinity (Alk) concentration, and C_w^4 is the toxicity (Tox) level. Each volume of stored substrate V_w can be selected as a substrate contribution to be transported to the ST. The selection is performed according to different volumetric possibilities (V_w^s, with $s \in \{0 \ldots, l_w\}$) that are determined as a multiple of a number (e.g., 1000) such that $1000 l_w = V_w$. The selection of each volumetric possibility is determined by the corresponding value of the binary decision variable, y_w^s, where $y \in \{0,1\}$, with $y_w^s = 0$ when the corresponding volumetric configuration is not selected, and $y_w^s = 1$ when it is selected. Note that for each waste generator w there are l_w different volumetric configurations in y_w^s, but only one is selected at a time, i.e., $\sum_{s=1}^{l_w} y_w^s = 1 \, \forall \, w \in \{1 \ldots, N\}$ (e.g., a waste generator with $l_w = 5$ would have five different volumetric configurations, but only one is selected at each optimisation iteration). The conveyance of the selected volumes implies a travel distance d_w with a social impact I_w and an economic cost x_w.

The blend of all transported substrate contributions constitutes the ST input. This input must be bounded by a certain set of restrictions, namely, the maximum acceptable volume V in the ST, the COD/TN ratio within the range $\left[C_{min}^2, C_{max}^2\right]$, the Alk concentration within the range $\left[C_{min}^3, C_{max}^3\right]$ and the toxicity level $\mathrm{Tox} < C_{max}^4$.

The objective is to minimise a cost function B, expressed as follows (note that the cost function is expressed as a quotient because the algorithm is intended to be maximized):

$$B = 1/\left\{\sum_{w=1}^{N} \sum_{s=0}^{l_w} y_w^s \, V_w^s T_w \left[\left(\sum_{c=1}^{3} F_w^c\right)\rho_q + \frac{\rho_x}{X_w d_w I_w}\right]\right\}, \qquad (1)$$

where y_w^s is the binary decision variable; V_w^s is the substrate contribution of generator W_w (in L); T_w is the sludge toxicity level (dimensionless); F_w^c is the set of coefficients corresponding to the substrate composition (dimensionless); ρ_q is the quality coefficient (dimensionless); ρ_x is the logistics coefficient (dimensionless); X_w is the unit cost (in €/km) of substrate transport; d_w is the distance between generator w and the anaerobic digester (in km); and $I_w = 1, \ldots, 3$ is a coefficient related to the social impact of substrate transport (dimensionless); the higher the value of I_w, the higher the social impact of the related route. The value of I_w is assigned qualitatively depending on different criteria e.g. route traffic density or proximity to pedestrian/sensitive areas where air pollution could impact human health. Hence, the use of routes involving critical areas—e.g., city centres or highly dense roadways—is related to a higher social impact factor (with a maximum value of 3). Consequently, a value for I_w is assigned for each sludge/substrate generator depending on its route to the ST.

The coefficients $\mathrm{F_w^c}$ $(\mathrm{c} = 1, \ldots, 3)$ and $\mathrm{T_w}$ are related to the role of the components ($\mathrm{C_w^c}$, with $\mathrm{c} = 1, \ldots, 3$) in the anaerobic process under the following conditions:

$\mathrm{F_w^1}$ is defined as the coefficient related to the potential biodegradation according to the COD content, following eq. 2. Such an equation has been drawn from [47], where it is used to quantify the organic content of the substrate and, hence, potential biogas production. Further calculations of biogas production have been made assuming a conversion factor of 0.268 m3 biogas/kg DQO (a parameter estimated from the current performance of the anaerobic digester of the case study and assuming minimal variations in retention time).

$$\mathrm{F_w^1} = 0.00001 * \mathrm{C_w^1} - 0.01 \qquad (2)$$

$\mathrm{F_w^2}$ is determined according to the ratio of COD/TN (eq. 3). Its value must be in the range 20–60, with a maximum value $\mathrm{F_w^2} = 1$ at $\mathrm{C_w^2}$=40. This equation is used in [47] to assign the optimum COD/TN ratio and penalise higher or lower ratios, which has been proven suboptimal for the anaerobic digester performance in the aforementioned reference.

$$\mathrm{F_w^2} = \mathrm{e}^{-\left(\frac{(\mathrm{C_w^2}-40)^2}{450}\right)} \qquad (3)$$

$\mathrm{F_w^3}$ is related to the alkalinity concentration (eq. 4), ranging from 3000 to 6000 g/m3 (which achieves maximum biogas production according to[47]). Then, the maximum value $\mathrm{F_w^3} = 1$ (i.e., optimum alkalinity) corresponds to $\mathrm{C_w^3}$=4500, which is related to the optimum alkalinity (high enough to prevent acidification but low enough to prevent salts precipitation), as used in [47].

$$\mathrm{F_w^3} = \mathrm{e}^{-\left[\frac{(\mathrm{C_w^3}-4500)^2}{8*10^6}\right]} \qquad (4)$$

$\mathrm{T_w}$ is a coefficient linked to the toxicity level. The Tox level is established according to the USEtox 2.1 toolbox toxicity estimation for a set of metals, expressed in total equivalent mg/L of lead (Pb). $\mathrm{T_w}$ has the highest values at the minimum toxicity levels. Hence, $\mathrm{T_w}$=1 for a Tox level=0, and $\mathrm{T_w} \cong 0$ for a Tox level ≥2.1.

$$\mathrm{T_w} = \mathrm{e}^{-\left[\frac{(\mathrm{C_w^4})^2}{0{,}6}\right]} \qquad (5)$$

The cost function presented in this work is adapted from [47], where the ACO algorithm is used for waste management optimisation in a similar fashion as here. The coefficient $\mathrm{T_w}$ is located outside the substrate biochemical characterisation to increase the importance of toxicity minimisation, which is a major risk for an anaerobic digestion operation [95] . The first term in eq. 1 is related to the quality composition of the substrate, and the second term in eq. 1 is related to the transport to the digester (the logistics term). The sum of both terms in eq. 1 is weighted by the coefficients ρ_q and ρ_x, allowing the assignment of different importance to each term. This enables stating whether the case study priorities are more focused on logistics or on maximising the anaerobic digester performance.

The cost function in eq. 1 is constrained by the decision variable y_w^s and the substrate characteristics (i.e., volume, composition, and toxicity level) that are acceptable for input to the anaerobic process.

Optimisation will provide a sequence that includes all the generators, where each generator is associated with its substrate contribution (including zero contribution) to the ST input. This optimised sequence may be interpreted as logistic planning based on the average travels per month: all transportation routes assume that a truck of 20 metric tonnes capacity is fully loaded with substrate from the waste generator, disregarding the truck waiting time before starting each route; once fully loaded, the truck would go directly to the waste receptor (assuming it always follows the same route). It is assumed that for all the co-substrate discharges made within a time frame equal to or less than the digestion hydraulic retention time (usually approximately 20 days) a blending effect would occur (otherwise, for the conducted case-study, equalisation tanks are available to hold different loads for a limited amount of time). On the other hand, the specific hour of the day where routes would start and finish has not been considered. This issue does not affect the solution of the algorithm, although it has been noted that this would be a significant issue for real-world implementation (due to potential social impacts for practitioners).

To construct a solution, the ACO algorithm follows the state transition rule defined by eq. 6.

$$p_{ws}^{m}(t) = \frac{[\tau_{ws}(t)]^{\propto}[\eta_{ws}(t)]^{\beta}}{\sum_{l=0}^{lw}[\tau_{wl}(t)]^{\alpha}[\eta_{wl}(t)]^{\beta}} \qquad (6)$$

where at iteration t, $p_{ws}^{m}(t)$ is the probability that the mth ant chooses the volume V_w^s; $\tau_{ws(t)}$ is the pheromone trail; α is the importance assigned to the pheromone trail; $\eta_{ws}(t)$ is the specific heuristic information; and β is the importance assigned to the heuristic information. The new heuristic information η_{ws}, defined in eq. 7, is used in the computation of a solution; the search seeks solutions by considering higher volumes, convenient substrate characteristics and shorter distances.

$$\eta_{ws} = \frac{V_w^s \sum_{c=1}^{3} F_w^c}{d_w} \quad (7)$$

The pheromone trail updated rule follows eq. 8 [49].

$$\tau_{ws}(t+1) = \rho\tau_{ws}(t) + \Delta\tau_{ws}^{best} \quad (8)$$

where $\tau_{ws}(t+1)$ is the pheromone trail at the beginning of iteration $t+1$; ρ is the persistence of pheromone in the trails (with $0 < \rho < 1$) corresponding to iteration t, and $\Delta\tau_{ws}^{best}$ is the amount of pheromone added to the trail of the ant that has achieved the best solution (B^*) at iteration t. The value assigned to this amount is defined in eq. 9 [47].

$$\Delta\tau_{ws}^{best} = B^* \quad (9)$$

6.3 Results

6.3.1 Case study

The case study included a network of 13 WWTPs which are part of the wastewater treatment system managed by Consorci Besòs Tordera (CBT), a public local water administration composed of 64 municipalities in four different regions of Catalonia (Spain) with a population of approximately 470,000 inhabitants. The area served by these WWTPs features a contrast between high anthropic-pressure areas (urban and industrial, relatively close to the metropolitan area of Barcelona) and other rural areas.

The sanitation network under study is composed of 12 WWTPs (W1-W12) that produce undigested sewage sludge and an additional WWTP with anaerobic digestion where the produced sludge would be treated. Figure 16 shows a map of the full wastewater system where the case study is located. Additionally, seven co-substrate generators from industries of the region have been identified by CBT practitioners as potentially viable substrates for codigestion (C1-C7). Due to regional legislation constraints, the maximum volume of codigestion with industrial substrates has been set at 9,000 L by day.

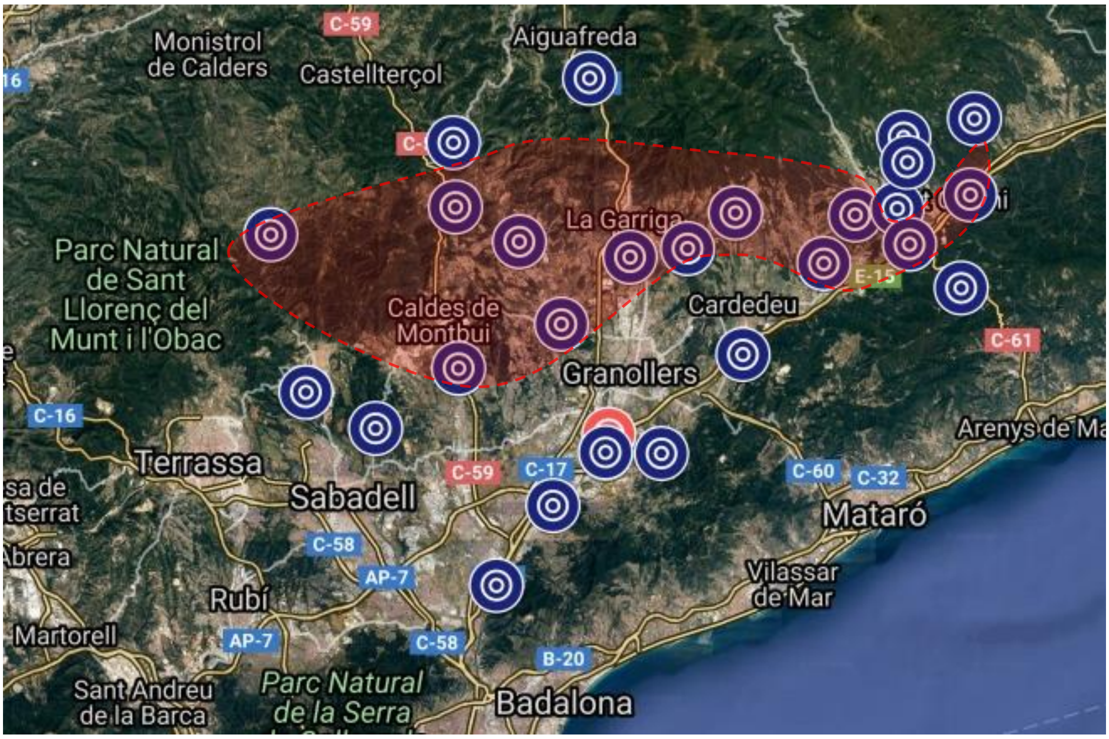


Figure 16. Map of the wastewater treatment system under study, where each dot corresponds to a WWTP. The specific sanitation network under study corresponds to the 12 dots under the red-shaded area (the WWTP with undigested sludge) and the red dotted WWTP (that corresponds to the receptor WWTP with anaerobic digestion)

6.3.2 Simulations methodology

The algorithm used in this work is programmed in Java. The simulations of the case study were performed with an HP EliteBook 840 G4 x64 using the OS Microsoft Windows 10 Pro and an Intel(R) Core(TM) i7-7500U CPU processor (2.70 GHz, 2904 MHz) consisting of two main processors and four logic processors.

Each simulation consists of 10 repetitions of the algorithm execution (their resulting values were averaged because of the probabilistic nature of the methodology), 500 iterations per repetition and 100 ants per iteration. All the repetitions start with a maximum pheromone trail on all the nodes to assign the same probability of selection to each node. The values used for the algorithm parameters are $\alpha = 1, \beta = 2$ and $\rho = 0.98$ ([48,49]).

The methodology was applied to a set of 19 substrate generators (12 WWTPs and 7 industrial substrate generators, which contain higher loads of organic matter than the 12 WWTPs and hence have higher potential for co-digestion strategies). The data corresponding to each generator are summarised in Table 23 and have been gathered as part of a real case study on the wastewater treatment infrastructure of CBT, a local water administration composed of 64 municipalities in four different regions of Catalonia (Spain) with a population of approximately 470000 inhabitants. In this area, 12 WWTPs (W1–W12 in Table 23) without anaerobic digestion have been identified, and characterisations of their sewage sludge have been performed. Additionally, seven external waste generators have been identified (C1–C7 in Table 23), whose substrate flows have been tested and validated as technically feasible for co-digestion purposes by CBT (by applying an internal co-substrate homologation process for WWTP anaerobic digestion).

A social impact factor $\mathrm{I_w}$ ranging from 1 to 3 was assigned to each route according to the corresponding social impact related to the route considered for each substrate.

Table 23. Waste generator dataset used for the simulations of the ACO algorithm. Each waste generator (W1-W12 and C1-C7) distance is related to the correspondent waste generator to the anaerobic digester receptor system. GR is referred to the sewage sludge produced within the same WWTP that includes the centralized anaerobic digestion system to be optimised.

ID	Vw (L by day)	COD (mg/L)	C/N	Alk (mg/L)	Tw (mg/L)	d (km)	X (€/km)	Iw
GR	359000	26900	20.3	2500	1.12	0	0	0
W1	27600	19900	17.8	4300	1.55	5.3	25.7	1
W2	47000	16900	20.6	3200	1.36	35.9	20.1	1
W3	46300	18600	19.4	10100	1.42	21.8	16.2	1
W4	20200	23400	15.6	3400	1.38	30.4	13.9	1
W5	38400	21100	17.9	4500	1.35	19.7	13.8	2
W6	34400	18800	14.0	3800	1.61	14.8	19.3	2
W7	13800	22600	15.3	2700	1.57	32.1	13.1	1
W8	4400	22100	15.2	1800	2.30	26.5	11.3	2
W9	10800	21700	15.1	5300	0.93	20.3	19.4	3
W10	9500	20400	15.5	2500	1.28	30	15.4	1
W11	17000	23300	14.8	7800	0.98	36.9	16.6	1
W12	6500	20100	16.5	3100	1.40	20.5	16.6	1
C1	9000	667400	42.5	250	0.01	15.9	15.4	1
C2	9000	497400	461.8	330	0.01	7	21.4	3
C3	9000	155900	3118.1	60	0.02	27.9	11.7	1
C4	9000	459100	274.1	660	0.10	16.2	12.6	1
C5	9000	657200	2330.6	630	0.01	52.8	11.6	1
C6	9000	266200	2832.4	20	0.01	56.1	10.4	1
C7	9000	262100	32768.4	110	0.01	5.6	19.4	1

In the approach presented here, one scenario is simulated based on the waste generator data in Table 23 and considering a single waste receptor. As specified in the case study section, the sanitation system under study is comprised of 12 WWTPs without anaerobic digestion and one additional WWTP with anaerobic digestion, and 7 cosubstrate generators. For all of those 19 waste generators (i.e. the 12 WWTPs without anaerobic digestion and the 7 cosubstrate generators) it is optimised the addition to the single anaerobic system of one of the main WWTPs managed by CBT, the Granollers WWTP (GR WWTP), whose own sludge properties have been introduced in Table 23. For that anaerobic digestion system, a volume constraint of 141 m3/d is used (corresponding to a retention time limit of 20 days).

The effect of the logistics on the optimised volume distribution is also assessed: two scenarios are simulated—O1 and O2, with 0 % and 50 % weight given to the logistics term ρx in eq. 1, respectively. Hence, in scenario O1, the optimisation is only focused on the quality of the blend—i.e., without considering the logistics impact on the optimal solution—whilst in scenario O2, the quality of the blend and the corresponding logistics are given the same importance to obtain the optimal solution.

Each simulation is repeated 10 times, consisting of runs of 100 ants and 500 iterations, since the ACO algorithm search is a probabilistic, iterative-based method.

Once the optimised volume distributions are obtained, further calculations are performed to characterise the corresponding logistics and the resulting anaerobic digestion balances. At this stage, the data of the variables detailed in Table 24 are obtained. It must be noted that the operating expense (OPEX) balance in Table 24 is obtained by considering integral waste management; hence, the related cost analysis considers not only the receiving system ST (i.e., the Granollers WWTP) but also the waste management costs related to W1–W12.

Table 24. Variables used for the characterisation of logistics and digester balance from the volume distribution. HRT is the hydraulic retention time; OLR is the organic loading rate.

Data description	**Units**
Digester operating data	
HRT	Day^{-1}
OLR	kg COD/m3·d
Biogas production	Nm3/d
Electricity production	kWh/d
Non-digested biosolids	kg/d
Digested biosolids	kg/d
Digester flows and quality composition data	
External sewage sludge addition	m3/d
External industrial waste addition	m3/d
Centralized non-digested sludge (treated anaerobically)	%
Logistic requirements for sludge centralization	Journeys/month
Logistic requirements for co-digested industrial waste	Journeys/month
Average COD of digester input	mg/L
Average ratio COD/N of digester input	-
Average alkalinity of digester input	mg CaCO3/L
Average toxicity of digester input	mg eq Pb/L
OPEX balance	
Dehydration system cost for external sludge generators	€/y
Non-digested sludge management cost	€/y
Non-digested sludge logistics cost (for centralized digestion)	€/y
Biogas valorisation benefits	€/y
Dehydration system cost after centralized digestion	€/y
Digested sludge management cost	€/y
Total cost-benefit analysis balance	€/y

The data obtained for the two optimised scenarios O1 and O2 are compared to those obtained for the additional non-optimised scenarios, for which the volume distributions of W1–W12 and the substrates C1–C7 are fixed. These scenarios correspond to the following: 1) Scenario M: manual volume distribution (according to expert knowledge criteria and the same volume constraints as in scenarios O1 and O2); 2) Scenario T: no volume constraint is considered (thus, all external sludge is processed by the receiving digester with no regard to retention time); and

3) Scenario C: control scenario according to the actual operating parameters of the receiving digestion system.

An additional constraint is considered, related to the valorisation of the biogas—set at 3800 Nm3/d of biogas, according to the current cogeneration capacity of the Granollers WWTP (which performs centralized co-digestion) for biogas valorisation. Thus, scenarios with and without this biogas valorisation restriction (referred to as biogas valorisation restriction, or BVR) are compared.

6.3.3 Scenario analysis

Volume distributions for each scenario are shown in Figure 17. Scenario C only involves the digestion of an external flow of 8000 L/day of industrial waste (C2), while scenario T involves the digestion of all the sewage sludge flows (waste generators W1–W12) but only the co-digestion of industrial waste C2. These pre-set scenarios are considered to compare the effect of absolute centralization without the potential biases caused by industrial high-organic-load external wastes. In addition, optimised scenarios O1 and O2 both involve the volume distribution generated by the application of the ACO algorithm to the set of 19 substrate generators. A summary of the results is presented in Table 25.

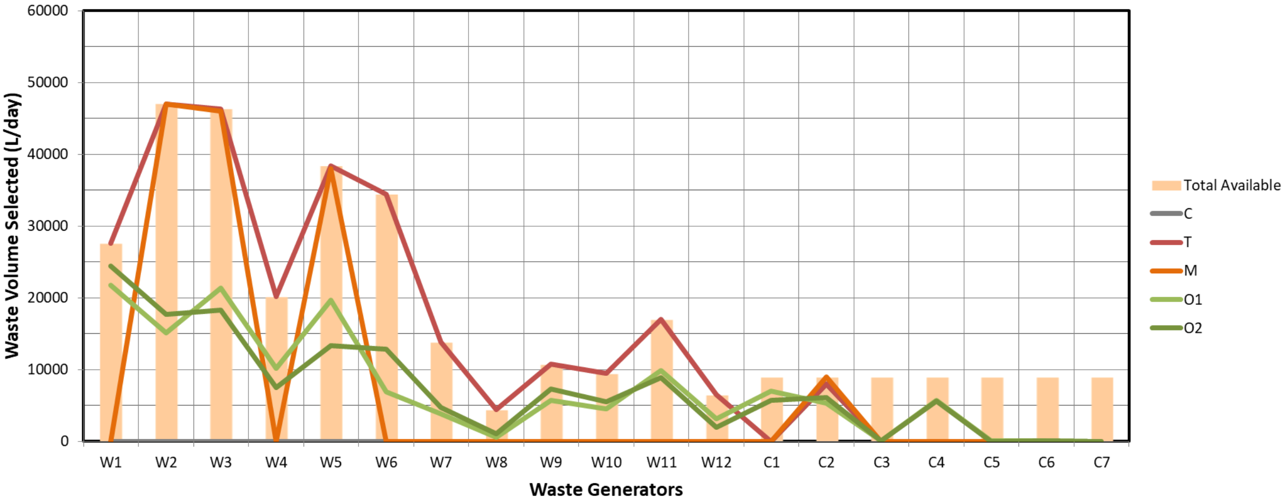


Figure 17. Volume distribution for each scenario (C: Current scenario; T: Total centralization scenario; M: Manual scenario; O1: Optimised scenario with 0 % logistic weight; O2: Optimised scenario with 50 % logistic weight) without BVR.

Table 25. Summary of results for each scenario, where O1 and O2 correspond to ACO-based optimisations and the C, T and M scenarios correspond to pre-set scenarios (current, total centralization and manual distribution scenarios, respectively).

Scenario	OPEX (€/y)	HRT (days)	OLR (kg COD/m3·d)	Biogas (Nm3/d)	Industrial Waste Dosage (m3/d)
without BVR					
C	-480000	27.2	1.2	3600	8
T	-93000	15.6	1.8	5100	8
M	-300000	20	1.5	4500	8
O1	-107000	20	2.1	6700	18
O2	-125000	20	2.0	6400	18
with BVR					
C	-480000	27.2	1.2	3600	8
T	-202000	15.6	1.8	5100	8
M	-354000	20	1.5	4500	9
O1	-350000	20	2.1	6700	18
O2	-346000	20	2.0	6400	18

As observed in Table 25, scenario T results in the highest (i.e., best) CBA balance but with a low retention time (HRT) trade-off. On the other hand, the optimised scenarios (i.e., O1 and O2) result in the highest production of biogas (and highest organic load rates) and the second and third best CBA balances while keeping the retention time at 20 days. Scenario M results in a balanced performance between the optimised scenarios and scenarios C and T.

Considering BVR in Table 25, almost no significant differences can be noted amongst the different scenarios: the lack of capacity to valorise all the produced biogas worsens all CBA balances except that for the current scenario (where biogas production is below the BVR). Moreover, little difference is observed between the M, O1 and O2 scenarios for all restriction combinations (the CBA balance is approximately −350000 €/year for the scenarios considered).

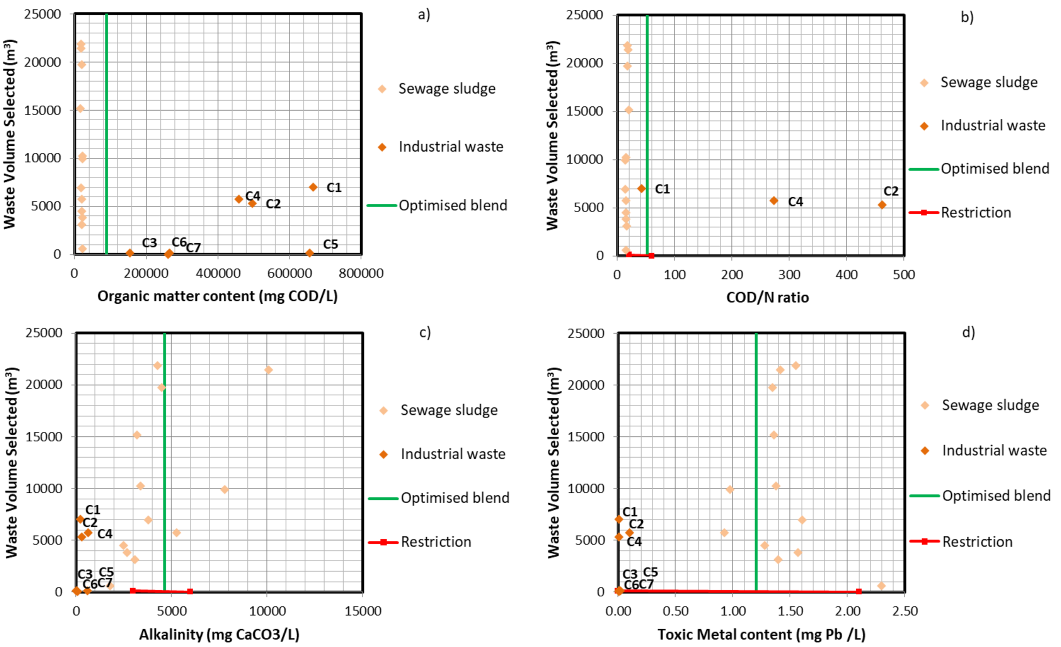


Figure 18. Waste generator volume selection according to a) organic matter content, b) C/N ratio, c) alkalinity and d) associated metal toxicity.

Figure 18 depicts the details of the optimisation results for scenario O1. To maximise biogas production, the algorithm optimises the combination of wastes with the highest organic content while keeping the restrictions on nitrogen content, alkalinity and toxicity.

For sewage sludge wastes (W1–W12), relatively similar organic and nitrogen contents are noted (approximately 20000 ± 2000 mg/L COD and 16 ± 2 COD/N ratio, respectively); however, the COD/N ratio (ranging from 14 to 20, as seen in Table 23) is below the low limit constraint of the ACO algorithm (set at 20). On the other hand, the COD/N values of the industrial co-substrates have much higher values and wider ranges (from 42 for C1 to 32700 for C7). The COD/N constraint is the limiting factor when composing the blend since the algorithm seems to prioritise industrial wastes with the lowest ratio of COD/N (C1, C2 and C4, as seen in Figure 18; C3, C4, C5, C6 and C7 are beyond the chart limits, but their contribution to the blend is minimal).

Regarding alkalinity and toxicity (Figure 18.c and Figure 18.d, respectively) industrial wastes show less alkalinity (300 ± 260 mg/L alkalinity) and less metal toxicity (0.02 ± 0.03 mg/L equivalent Pb) than sewage sludge (4000 ± 2400 mg/L alkalinity and 1.4 ± 0.3 mg/L equivalent Pb). Hence, it may be noted that from a toxicity perspective, these industrial substrates would be safe for co-digestion strategies (although their high COD/N ratio limits their usage due to the COD/N ratio restriction over value 60).

6.4 Discussion

The employed ACO algorithm allows an optimised logistic planning proposal to be obtained in terms of the average volume extracted from each waste generator. This, together with data from the case study, allows average travels per month, biogas production and the resulting OPEX balance to be estimated. Other existent optimisation algorithms regarding anaerobic co-digestion that were introduced previously in this paper have been focused on separate aspects of anaerobic co-digestion (always with the objective of maximise biogas production): in [83], the focus is placed on linear optimisation of the feed composition through the detailed conversion routes of each compound of the feed (e.g., carbohydrates, lipids, proteins); in [84], linear optimisation of the feed is also performed, taking into account the potential effects of the pretreatment technologies, so the output also considers a technology assessment about substrate pretreatment processes; and in [96], the focus is to study the anaerobic digestion dynamics of the main metabolic reactions and the biochemical transformation pathways for various organic compounds, so that it allows a deeper analysis of the transition from mono-digestion to co-digestion (since such transitions always depend on the type of microbiota in the digester and their adaptability to the organic load increase). Additionally, algorithms focused on logistic optimisation already exist, e.g., in [93], where an ACO algorithm is applied to optimise truck routes (but not considering other properties of the transported materials, such as the biochemical properties of sewage sludge in the case study of this work), or in [97], where GIS-based optimisation is carried to address faecal sludge logistics. The novel ACO algorithm developed in this work is an approximation to tackle most of the aforementioned issues from a holistic perspective (such as considering logistics, volume distribution, and cosubstrate blend optimisation, working within the operative restrictions of volume, alkalinity and nitrogen loading).

Without BVR (Table 25), the optimum scenario is O1, despite having a slightly lower CBA (−107000 €/y) than scenario T (−93000 €/y). This difference in CBA is because all variants of scenario T consider the total centralization of all the non-digested sewage sludge (from W1–W12), and hence, the HRT is drastically reduced to approximately 15 days. Since these operation conditions are at the edge of conventional and convenient anaerobic digestion management conditions, this strategy implies a relatively risky shift in operation conditions. In addition, less efficient biogas production, a decreased buffer capacity of the digester in the case of metal toxicity, and an increased risk of acidification would be expected. The precise motivation of the optimisation problem (approached herein by the ACO algorithm) is the need to set a limit on the acceptance of external wastes to avoid these undesired conditions of operation.

For the manual distribution approach, as observed in Table 25, the pre-set scenario M results in a lower CBA than the optimised scenarios O1 and O2 (without BVR, scenario M has a CBA of −300000 €/y, while scenarios O1 and O2 have CBAs of −107000 €/y and −125000 €/y, respectively). This is because scenario M adds less industrial, high-load organic waste (from 8 to 18 m3/d) and thus allows less production of biogas (4500 Nm3/d, in comparison to the 6400–6700 Nm3/d of O1 and O2). However, the O1 and O2 scenarios allow for more biogas production than the manual scenario since the optimisation process allows for the control of critical factors such as alkalinity and the COD/N ratio. The monitoring of these parameters is paramount to avoid acidification of the digester, which may have an important impact on its performance and may be avoided using appropriate diagnosis and optimised blending strategies, such as the one presented here.

On the other hand, potential legislation and other policy-based limitations on the addition of industrial substrates (such as those corresponding to C1–C7) have been identified, but they have not been considered in this study. If enacted, these additional restrictions could reduce the effectiveness of a co-digestion strategy below its full technical potential, as shown by the ACO algorithm approach.

Regarding the impact of the logistic term on optimisation in the CBT case study, minor differences are observed between scenarios O1 and O2 (as seen in Table 25). Scenario O2 shows a slightly lower CBA balance than O1. Hence, in this particular case, increasing the weight of the logistic term to 50 % of the cost function does not provide a better CBA balance. This result may indicate that external substrate waste generators with higher biomethanisation capacity are geographically closer to the anaerobic digester receptor ST (Granollers WWTP) than those with less potential to produce biogas. Note that the case study involves waste generators with logistic distances below 30 km. Without loss of generality, for different scenarios with higher logistic distances, the logistic term might be more significant, but it is not the case here, where the distance between co-substrate generators and receptor do not seem to be significant for optimisation purposes. This logistic term, however, could be significant for the present case study if stronger restrictions and/or penalties would be considered regarding, e.g., social impact factors, CO2 emissions penalisations, or a different geographic configuration of external substrate generators.

A comparison of the scenarios with and without BVR shows that lower differences are observed with BVR in the CBAs of scenarios M, O1 and O2. This result indicates that the added value of the optimised scenarios comes particularly from those scenarios with a higher ability to produce biogas, i.e., when biogas valorisation is not constrained, as with BVR. Hence, the limitation on biogas valorisation blocks most of the benefits obtained from the application of optimisation strategies for co-digestion.

Accordingly, to maximise the CBA of the co-digestion strategies, the capacity of biogas valorisation should be increased to 7000 Nm3/h for the Granollers WWTP, and the volume distribution in scenario O1 should be followed; under these conditions, industrial co-substrate volume addition would comprise 18 % of the total input to the digester, and a potential cost reduction of 77 % in CBA could be obtained (from −480000 €/y for scenario C to −107000 €/y for the proposed scenario O1).

It may also be noted that optimal digester operation is paramount to achieve good performance; such optimisation can be achieved by using tools such as the one in [82], and significant operational costs may be saved when optimising the blend, as detailed here, and when assuring optimal digester conditions, e.g., via properly optimising alkalinity, toxicity and COD/N while maximising the organic content and thus biogas production. The ACO algorithm presented herein allows for the optimisation of the co-substrate blend and logistic planning.

Hence, implementation of this tool in actual installations should allow significant co-digestion performance improvement, with a potential reduction in waste management costs of 77 % for the 13 WWTPs involved in the case study. Moreover, if this tool is used together with an on-line digester monitoring and diagnosis system, digester stability is assured, and possible risks such as digester acidification or intoxication will be minimised.

6.5 Conclusions

In this work, the optimisation of the co-digestion strategy in a real case study in the waste management sector is considered by means of the implementation of an ACO algorithm in a novel fashion, considering both the quality and the logistics of each co-substrate, obtaining an optimised planning strategy for a real multi-plant case study. The main conclusions of this study are as follows:

Logistic-related parameters of each waste generator (i.e., distance, cost and social impact) have been adapted from the approach presented in [98], which was originally conceived for sewage sludge biochemical properties.

The results obtained show how an increasing logistics weight in the optimisation provides a lower expected distance (hence, lower transportation costs) and lower social impact factors, even though this does not have a significant impact on CBA in the case study considered.

An optimised blend of sewage sludge with an 18 % volume co-substrate is achieved, allowing an increase in organic matter content of +188 %, a C/N ratio upgrade from 16 to 59, a reduction in toxicity from 1.61 mg Pb/L to 1.36 mg Pb/L and a potential waste management cost reduction of 77 %.

The significant improvement from the manual scenarios to the optimised scenarios when no limit on biogas valorisation is imposed suggests the importance of optimised blending to attain improved performance.

Further work may include the consideration of multiple anaerobic digesters as sludge and co-substrate receptors to increase the current limit on biogas valorisation (i.e., when the blend optimisation process yields better performance) and to optimise the current overall potential of CBT for co-digestion. In addition, implementing methodologies to objectively quantify the social impact factor would allow better characterisation of the logistic impact of each substrate generator.

Chapter Seven

General discussion

7.1 Discussion of case study properties and applicability

The case study is set within a region of Mediterranean climate, with high anthropogenic impact. As a result, the local environment is relatively sensitive, and the WWTPs of CBT are managed over the average efficiency of EU WWTPs. Also, probably due to the characteristic orography of the region, sanitation is relatively decentralized when compared to Europe and USA WWTPs (which generally have smoother terrains, allowing for easier implementation of centralized sanitation systems). This decentralization implies that there is higher proportion of small WWTPs where eco-innovation can prove more challenging due to economics of scale; besides, they also prove a challenge to WWTP management, thus requiring more efficient communication and organisation with the entire CBT environment. Also, the local differences between each of the 23 sanitation systems comprised within CBT environment (while some are more rural, others are more urban and industrial) increases the complexity of the task of simultaneous management of multiple WWTPs.

However, most of the CBT WWTPs have already a good performance for nutrient removal and the biggest WWTPs have implemented anaerobic digestion, which enables centralized anaerobic digestion of undigested sewage sludge. That strategy allows an increase of biogas, and simultaneously reduces the number of sludge cake producing WWTPs from 16 to 4 (LL, MT, GR and RV WWTPs, the ones with anaerobic digestion). Besides, digested sludge cake has more advantages than undigested sludge cake: it enables valorisation by direct use as agricultural fertilizer (if all additional requirements are met, as set by the corresponding local authorities).

As shown in Figure 10, in terms of energy efficiency CBT WWTPs are around the average, although most of CBT WWTPs correspond to treatment capacities below 5000 m^3/day and energy efficiency below that threshold has higher variability (due to the many ways each WWTP is build and operated, in contrast to relatively standardized procedures for bigger WWTPs where the best available technologies are mostly applied to increase energy savings).

The use of mass balances detailed in Chapter 4 has provided useful insights about the potential added value of processes such as anaerobic digestion: while undigested sludge carries over approximately the 60% of influent organic matter, anaerobic digester extracts half of it (or the 30% of influent organic matter) into biogas. Thus, only the process of mesophilic anaerobic digestion transforms half of the energetic content of sewage sludge in an energy carrier with such potential as biogas. However, an important fraction of organic matter (about a 30% of influent wastewater total elemental carbon) is oxidised through conventional activated sludge biological processes of wastewater depuration; water line processes such as High Rate Activated Sludge (HRAS) or Upflow Anaerobic Sludge Blanket (UASB) allow avoiding such quantity of carbon oxidation, transferring that carbon directly to the sludge (thus, enriching sewage sludge organic content) or directly to biogas. These processes aren't currently implemented in the developed tools, so the expansion of the technology library for simulation should be a direction for future research.

Regarding sewage sludge management, waste-to-energy is an increasingly attractive process: this is because it allows transforming all the sewage sludge organic matter in energy (bypassing the transformation in energy carriers, although some processes such as pyrolysis enable production of biochar and biofuels). On the other hand, fertilizer use of sewage sludge has increasing restrictions and composting suffers from capacity overloading (and, consequently, price increase). Thus, there are significant uncertainties related to which sewage sludge management pathway will be more favoured by new policies or by the waste management market evolution. As a result, smart tools as the developed in this work can prove useful to perform quick assessments and preview the impact of the different possibilities.

Also, successful eco-innovation has different bottlenecks from both economic and social perspectives. These bottlenecks can be (partially) addressed by means of data and information management, such as decision support systems and further ad-hoc methods. Overall, the CBT environment shows promising properties to study and further boost circular economy implementation (in the field of sewage sludge valorisation); so, the application of a generic methodology of DSS development to address the case study problem has allowed obtaining a process simulation and modelling approach that has been used as a scenario based DSS tool. On the other hand, the systematic analysis of the CBT environment and its sanitation systems led to the proposal and design of an optimisation tool for centralized anaerobic digestion. Both of these solutions can effectively help surpassing some of the present and future challenges of sewage sludge waste valorisation. Plus, their design has been intended to be replicable with other sanitation systems.

7.2 Discussion of applicability of DSS tools

Modelling is a well-known method to gather insight for systems with different types of processes. Scenario simulation is an essential method used by decision-makers and other professionals alike to preview the behaviour of a certain system in different situations e.g. using different configurations. However, the undesired effect of uncertainties may jeopardize the reliability of such simulations, being a significant concern for decision-makers. Thus, when assessing a decision it is important to consider the array of possibilities. For that purpose, DSS tools are usually based on scenario simulation. Coupling both scenario simulation and process modelling, for the case study of sewage sludge valorisation within WWTPs, the tool developed in this work combines both methods: it allows assessment of an array of possibilities while simultaneously gathering insight of the processes involved.

However, intentional design is crucial to ensure applicability of the method, as pointed in the Introduction section. It is the reason that all work conducted has been focused to validation with real case studies and that feedback from practitioners has been collected along the different phases.

The use of KPIs is intended to summarize information and gather insight from the simulation output. Besides, using time-series as data input of the modelling and scenario simulation DSS tool presented in this thesis allows time-dependant analysis. Precisely, that feature can prove useful for dynamic systems with significant seasonal variabilities such as WWTPs: for example, thermal balance, biogas production, pollutant load of wastewater and other variables can provide additional information when their correspondent profiles over time are studied.

Overall, the capability to prepare, model and simulate scenarios with a smart tool such as the presented SIM-SAD enhances the process of decision-making. With the present and future challenges overseen with the SWOT analysis in the Case Study section, quick adaptation to new WWTP management and operation conditions is essential. The presented SIM-SAD tool, thus, contributes to supplying the lack of smart tools available for the case study, enabling further processing of information and data available regarding the WWTP and exploiting knowledge.

7.3 Discussion of applicability of centralized anaerobic digestion optimisation tools

Anaerobic digestion is a key process of sewage sludge valorisation (and, thus, circular economy implementation, contributing to achieving sustainability) and it is widely implemented. However, frequently these processes lack optimisation, so that's the reason there has been much research the last decades to increase its performance, based on biochemical modelling and, overall, developing tools to control and even predict biogas production and keep a balance of the most significant compounds that may affect digestion performance: keeping a certain level of alkalinity prevents acidification; keeping a low metal content minimizes risk of inhibition (which can cause a biocide effect, thus disabling any effect of the digestion process); on the other hand, keeping a ratio of carbon nitrogen above 20 (or, conversely, high amounts of nitrogen in respect to biodegradable organic matter) avoids the production of ammonia mid-process, thus minimizing the risk of inhibition by that substance; and keeping a ratio of carbon nitrogen below 60 (or, conversely, too high amounts of organic matter) helps keeping the equilibrium of alkalinity.

Note that an excess of organic matter, although it would seem beneficial because it allows processing more organic waste and producing more biogas, can derive in significant reductions of alkalinity. Thus, operation of anaerobic digestion is not a simple task, especially when codigestion of various substrates with different properties is performed. As a result, optimisation of codigestion has been already broadly addressed by development of other tools.

The approach followed in this thesis regarding codigestion process improvement revolves around the concept of centralized anaerobic digestion optimisation. For that purpose, optimisation method based on the ACO approach has been applied successfully to optimize the blend of a WWTP with sewage sludge and other external organic wastes. This is a promising tool for cases such as that of CBT environment where multiple WWTPs are close to each other and the biggest ones have anaerobic digesters with available capacity. However, the combinatorial complexity of optimising the blending form undigested sewage sludge from 12 WWTPs and external organic waste form 7 industries requires the use of techniques such as the one presented in this work. As shown in Chapter 6, the use of such a tool for optimisation of centralized anaerobic co-digestion allows proposing new pathways of sludge management that provides potential cost savings of up to 77% in waste management of the sanitation systems. Although the applied methodology has further research potential, it has already provided with significant and promising results. This proves a key added value of the thesis to the optimisation of waste management in sanitation systems and, ultimately, enhancing the implementation of circular economy related processes within such sector.

7.4. Discussion of the thesis impact

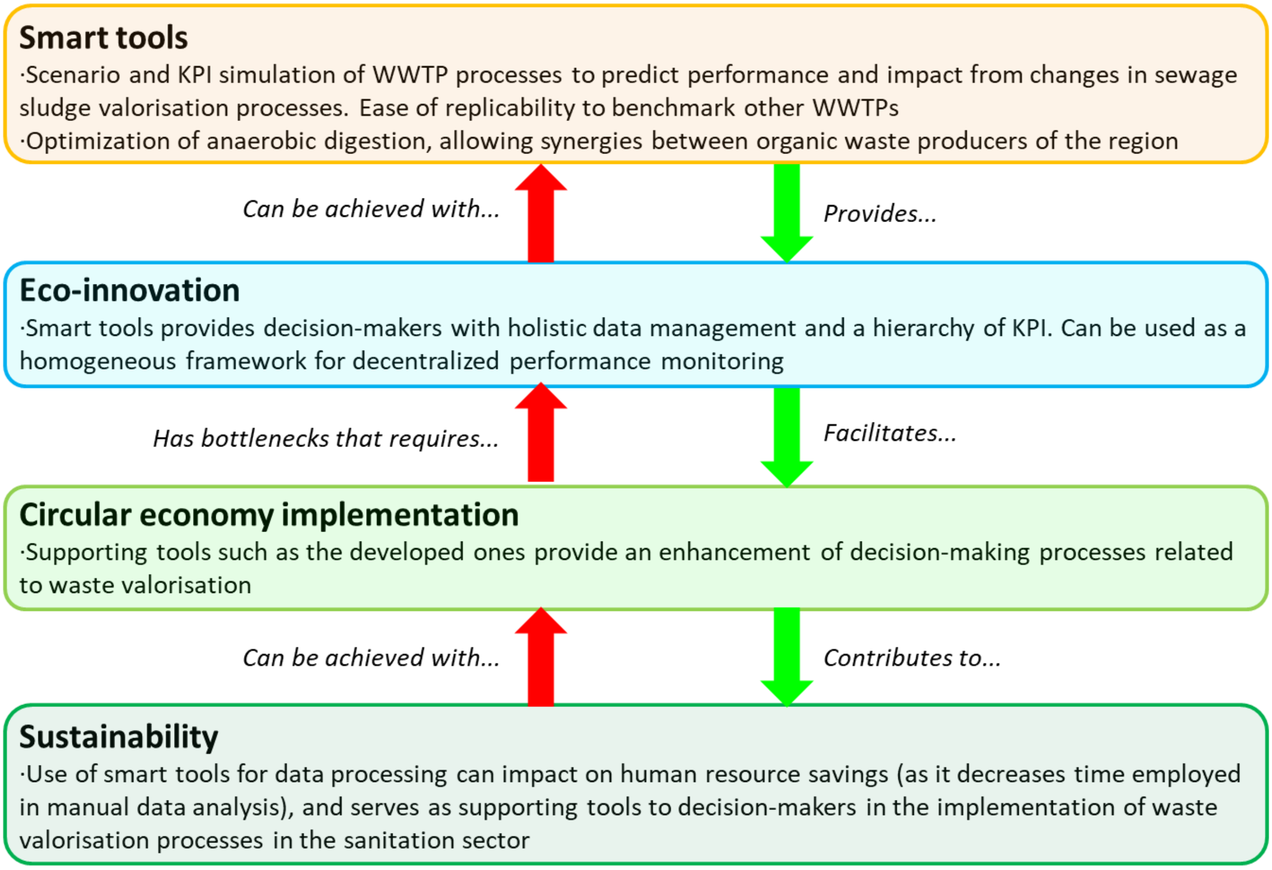
As stated in the Introduction section, sustainability requires circular economy. At the same time, circular economy is an eco-innovation. Different bottlenecks have been identified towards implementation of eco-innovation (and other specific challenges of circular economy). The use of smart tools to improve the chances of implementation of eco-innovation is a promising strategy, as demonstrated with the case study of the thesis, which revolves around waste valorisation in sanitation systems.

The application of the DSS-development method has allowed developing an innovative smart tool which focuses on scenario simulation of processes within a WWTP, using KPI sorted in a hierarchy. Each WWTP is a highly complex system, generating significant amounts of data. Besides, since each WWTP has a different configuration the decision-making process increases in complexity because practitioners must combine both qualitative and quantitative information (that is, data and knowledge). In this sense, the developed SIM-SAD tool provides practitioners with an additional supporting framework to process measurable data and predicts the degree to which changes in the WWTP configuration may affect its performance and impact to the environment. As shown in Chapter 5, the use of the tool has shown satisfactory results to benchmark a same WWTP considering different waste valorisation pathways, each with their own set of indicators to provide with a holistic preliminary analysis to decision-makers and practitioners alike.

On the other hand, conceptualizing the synergy of the combination of local sanitation systems as connected units by means of centralized anaerobic digestion has led to the development of a blend optimisation tool for anaerobic digestion, applied with both undigested sludge and external organic waste. This is a significant step towards circular economy because it would facilitate the valorisation of external organic waste from other industrial sectors within the sludge treatment line of the WWTPs. Although different optimisation tools have been developed before, the approach presented in the thesis includes a term to consider logistics in order to optimise the blend. That has enabled a results discussion considering not only the biochemical properties of each waste contribution, but also the impact of logistics. That is a significant step towards holistic sewage sludge management, because the impact of logistics is relatively hard to quantify, due to the ad-hoc nature of each case study and many variables that may affect the quality of a transport route: the state of infrastructure, road density and proximity to urban areas or other areas sensitive to traffic pollution or noise are just some examples of the complexity regarding impact of logistics.

Thus, the development of such tools can be considered an eco-innovation because they thrive to enhance the holistic management of WWTPs. Furthermore, they provide a homogeneous framework where practitioners from different WWTPs could benchmark their respective performance and impact. Precisely, the fact that the CBT sanitation environment is decentralized and that is shows significant geographical differences amongst each system has been traditionally a challenge for holistic management of the whole environment. However, the use of the presented smart tool SIM-SAD, as a homogeneous decision-making platform that can be used for any WWTP, can help towards achieving a higher degree of communication in such a decentralized sanitation environment. Since eco-innovation implementation usually involves multidisciplinary concepts, data and information aggregating methods such as DSS development are useful.

Overall, these tools can improve circular economy implementation by providing practitioners and decision-makers with supporting tools focused on data management and simulation of waste valorisation processes within WWTPs. Simultaneously, they provide with a homogeneous framework to facilitate holistic management of the sanitation system and potentially reduce human resources required to manually analyse and process data. Since sustainability revolves precisely around the wiser use of both tangible and intangible resources (such as waste valorisation and increasing the efficiency of the decision-making processes), the developed tools in Chapters 5 and 6 can provide indirect but clearly positive contributions to increase the degree of sustainability within the sanitation sector. Here relies the innovation and impact of the thesis presented. Figure 19 summarizes the thesis impact and contribution of the developed methodologies applied within the sanitation sector.


Smart tools

·Scenario and KPI simulation of WWTP processes to predict performance and impact from changes in sewage sludge valorisation processes. Ease of replicability to benchmark other WWTPs

·Optimization of anaerobic digestion, allowing synergies between organic waste producers of the region

Eco-innovation

·Smart tools provides decision-makers with holistic data management and a hierarchy of KPI. Can be used as a homogeneous framework for decentralized performance monitoring

Circular economy implementation

·Supporting tools such as the developed ones provide an enhancement of decision-making processes related to waste valorisation

Sustainability

·Use of smart tools for data processing can impact on human resource savings (as it decreases time employed in manual data analysis), and serves as supporting tools to decision-makers in the implementation of waste valorisation processes in the sanitation sector

Figure 19. Summary of thesis impact and contribution: from sustainability to the need of smart tools, and how they contribute to the latter, in the sanitation sector.

Regarding the concept of circular economy, it usually involves valorisation of waste produced near to the location where it was produced. However, strictly speaking, circular economy would imply that the waste produced should return to the place where it came from: for instance, due to the globalised food market, significant amounts of food come from other countries (and even other continents); strict application of circular economy would mean the correspondent portion of waste generated should return to such far away locations. However, logistics are a heavy issue, a bottleneck towards achieving true circular economy. Precisely, the motivation behind struvite production from sewage sludge return liquors is the capability to produce a concentrated agricultural fertilizer that might me more economically feasible to commercialise between far away locations, in an attempt to return that material to its true origin. In contrast, the current concept of circular economy is a sort of circular economy “of proximity”; it means that both its concept and their related eco-innovations have been used to boost sustainable development in different regions through building local business models orientated to local and eco-innovation based processes. Ironically, that local circular economy concept, despite it dissents with the current global market, contributes to building value chains more resilient to global changes or threats, such as the case of the unprecedented SARS-COV2 pandemic that has led to severe economic hindrances of global markets. Besides, note that in this thesis the focus of circular economy was limited to the sanitation environment, although to fully achieve it in the geographic region it would be required to tackle all the variety of wastes not only from the sanitation sector but also from the other human activities of the area.

Aside from the concept of circular economy, there are other concepts whose perception must be revised: that's the case for the concepts "waste" and "disposal". Conventionally, both terms have negative perspective; nevertheless, throughout the thesis they have been used. The point to discuss here is that despite they have negative connotations; they should still be used in favour of new, positive, optimistic connotations. Truth is that instead of "waste" and "disposal" other terms are favoured, such as "substrate" or "valorisation" when the discourse revolves around sustainability and circular economy. It is relevant to note that both conventional and new "positive connotation" terms have been used; that is because in order to favour a healthy discussion it is important to include also negative connotation terms. This way, myths, taboos and biased connotations assigned to each concept related to waste management can be deconstructed easier, hence contributing to a more rational social environment (which, as mentioned in the Introduction section, it is also a fundamental pillar to achieve sustainability).

Finally, it is important to highlight, again, the relevance of data and knowledge. These are two separated sources of information (the first being more quantitative, and the second more qualitative). There already exists many methods revolving around the use of data to extract value from it (data analytics methods), but knowledge is either considered as contingent to interpretation from data or directly forgotten. That is why, in the modern context of organisations with high amounts of data and data processing methods that generates knowledge, knowledge management systems are also an essential counterpart not only to store new information obtained from data observation, but also to avoid decay and loss of knowledge of any source. Furthermore, research projects such as the one carried within this thesis' framework, where multiple data and information sources are available from multidisciplinary fields, requires first to collect and handle all that information before even starting to apply the methods and develop solutions. Thus, before attempting to valorise waste, data and knowledge must be valorised first.

Chapter Eight

Conclusions

The key driver behind the present thesis is sustainability. That concept has attracted much attention from professionals of different sectors, because of its appealing towards a future where economy, society and environment coexists in relative harmony. Yet, it is an abstract concept itself. This thesis follows through the strategic vector of circular economy, and from there it is applied to the sanitation sector.

The sanitation sector has a significant potential for circular economy potential because it is a Water-Energy-Food nexus and it provides an essential service to humankind. Besides, it comprehends certain processes that can convert organic matter into energy carriers, such as anaerobic digestion (which is a highly studied process during the last decades). However, different bottlenecks and challenges have been identified towards implementation of circular economy within sanitation systems (in the form of sewage sludge valorisation). To enhance eco-innovation processes such as the implementation of sewage sludge valorisation in WWTPs, the present thesis develops and tests novel new smart solutions to enhance the decision-making and assessment processes.

Such tools have been envisioned from the perspective of the generic method of DSS development due to its capability to provide value to significant amounts of heterogeneous data and knowledge. That has proven a useful method for such a multidisciplinary sector such as sanitation, where many processes are involved. It is important to highlight that the application of such method has allowed to perform an exhaustive analysis of the case study where the developed tools are tested, before the testing itself, to improve the intentional design of the solutions and maximize their fitting to the drivers of the sanitation sector. Besides, the same case study has been used to develop a novel method for centralized anaerobic co-digestion optimisation, based not only in biochemical properties of sewage sludge, but also on logistic properties of the route of each waste generator involved in the centralized digestion process, by means of Ant Colony Optimisation methodologies.

The case study corresponds to the CBT environment, a public local water administration in charge of the management of 23 sanitation systems. It has been observed that this environment, since it is located in a Mediterranean climate, has major risk of forest fire and water scarcity, so the freshwater masses of the corresponding region are relatively sensitive. Plus, there is a high anthropogenic impact for the most part of CBT environment due to highly dense urbanisation and industrialisation at the bottom of the geographical area. CBT WWTPs have shown performance around the average of European and USA WWTPs, and together they form a combination of small and medium sized WWTPs, where the bigger ones have anaerobic digestion. That makes it a convenient case to apply centralized anaerobic digestion strategies.

Also, a novel DSS KPI-based tool -called SIM-SAD here- has been developed in order to provide insights for the sanitation installations management at WWTP level. The proposed SIM-SAD tool has allowed estimating the potential impacts of various combinations of technologies according to the case study, which have been modelled and simulated, and the outcome of these simulations has been provided in a designed hierarchy set of KPI in order to summarize the results and help the technology assessment process. On the other hand, a novel optimisation strategy for centralized anaerobic co-digestion has been developed, showing very promising results at the pre-implementation stage and allowing exploiting synergies with external organic waste generators. These specific smart tools have allowed overcoming some of the mentioned challenges to implementation of sewage sludge valorisation. Nevertheless, effectively achieving implementation of circular economy and similar eco-innovation initiatives requires more exhaustive data and knowledge valorisation through additional tools: thus, improved online data monitoring with centralized supervisory infrastructure and knowledge management systems are also required.

Contributions

The contributions of this thesis are mainly focused on enhancing the decision-making and assessment processes of implementation of circular economy in WWTPs. Concretely, this has been achieved through the development of a novel DSS KPI-based tool, which has been designed to simulate scenarios and manage the provided information by means of a hierarchical time-series based set of KPIs, with the aim of facilitate the analysis of the considerable and heterogeneous amount of information provided by the simulator, in order to assess the performance of the overall chain of WWTP processes implemented. Testing of this tool with the case study here has demonstrated that it provides very useful insight for the assessment of different process configurations of sludge valorisation in WWTPs. This constitutes a framework for further discussion for practitioners in order to preview the impact of different WWTP technology setups to the performance of the plant from a holistic perspective. On the other hand, a novel method for the optimisation of the centralized co-digestion in a real sanitation system has been also developed, showing promising added value for its final implementation in the actual case study, in which it allowed at a simulation stage successfully maximising the biogas production while respecting a set of constraints related to the real system, namely: available volume, impact of each route, metal toxicity and concentration of nitrogen and alkalinity. For the case study, tool testing results have provided potential cost savings of up to 77% in waste management of the sanitation system. Besides, since practitioners usually operate each WWTP independently, manual centralization of co-digestion adds an increased management difficulty. Nevertheless, the developed tool for optimisation of centralized co-digestion also helps overcoming this implementation bottleneck.

Directions for future research

Aside from the milestones achieved in this thesis, further work related with this thesis is required to successfully implement the developed strategies at full-scale and within the daily routines of wastewater management. First, to assure that the SIM-SAD provides reliable outcomes, it is important that uncertainties to the processes and technologies involved associated are deeply acknowledged and understood by the user. Data quality must be maximised and uncertainty sources exhaustively tracked to assure reliable tool outcomes. Also, the application of further data mining processes to the output of the simulation can provide with more refined discussion framework for decision-makers.

Regarding the optimisation of centralized anaerobic co-digestion, to further increase the applicability of such method to more complex case studies it is necessary to develop a multi-receptor version of the current algorithm. This way, the same method could be applied to optimise simultaneously the centralization of co-digestion to a set of digesters in different locations. Data quality and management of the associated uncertainty is also crucial to assure a reliable implementation of the optimisation method. Furthermore, once implemented such method, monitoring of digester performance would provide with valuable data to further refine the method and serve as a data validation framework.

Chapter Nine

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Chapter Nine

Annexes

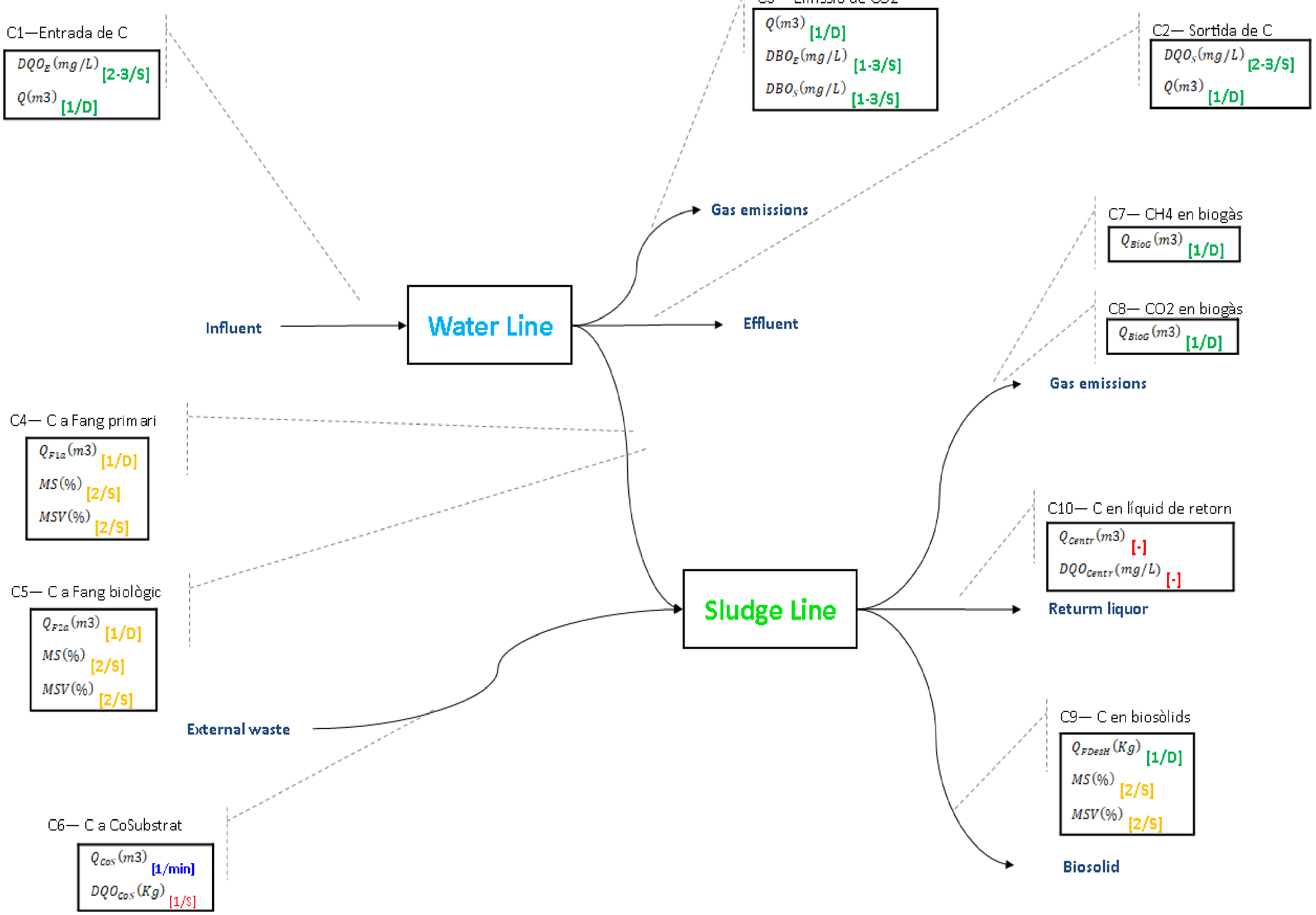
Annex 1

WWTP tag and correspondent municipality

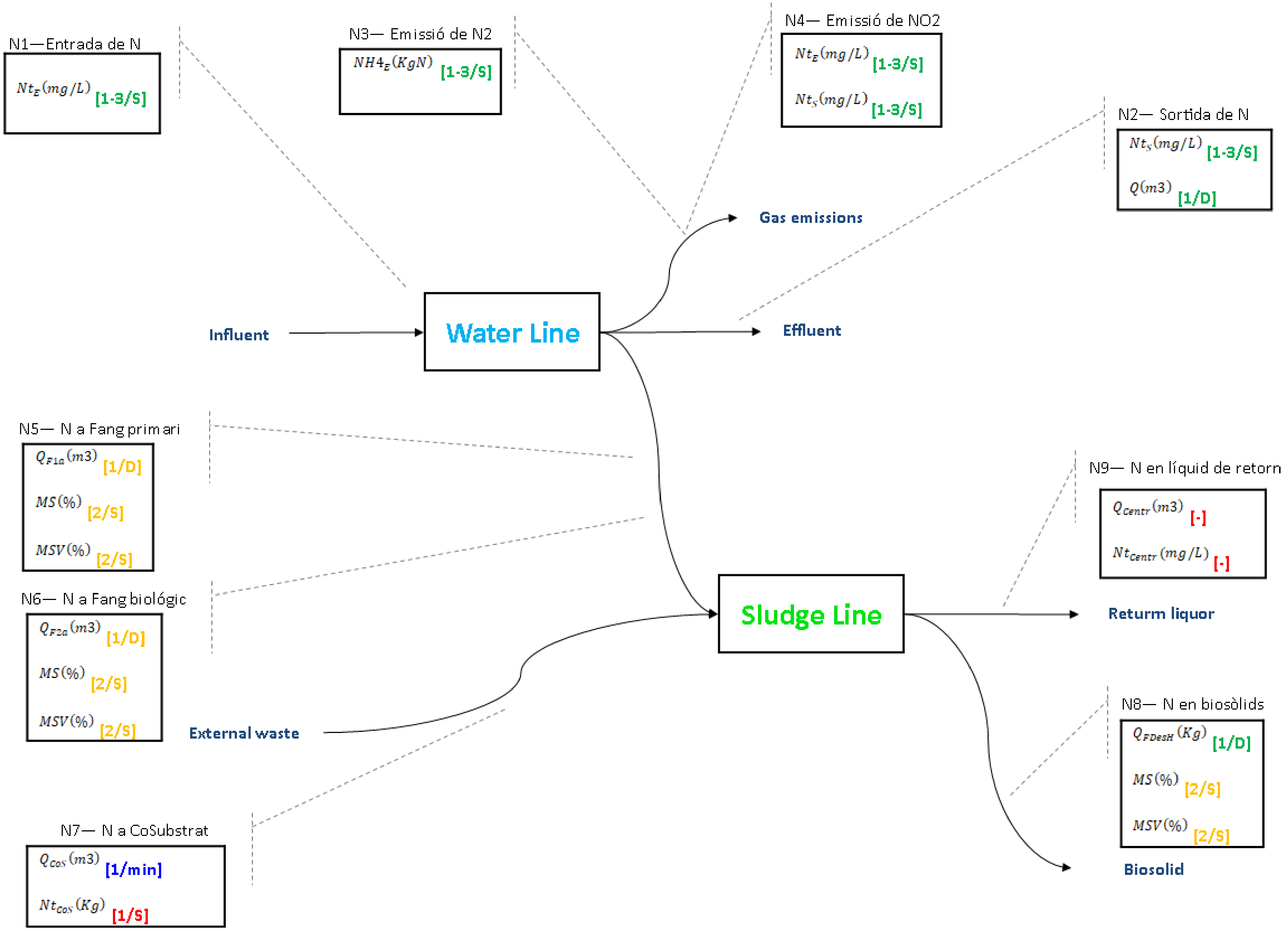
Tag	Name of correspondent main municipality
LL	La Llagosta
MT	Montornès
GR	Granollers
RV	La Roca
VV	Vilanova Vallès
CV	Castellar Vallès
CMB	Caldes de Montbui
SC	Sant Celoni
G	La Garriga
SER	Santa Eulàlia Ronçana
SMP	Santa Maria Palautordera
C	Congost
SAV	Sant Antoni Vilamajor
SFC	Sant Feliu Codines
SQS	Sant Quirze Safaja
CS	Cànoves-i-Samalús
BR	Bigues-i-Riells
CR	Can Ram
CC	Can Canyameres
CP	Campins
M	Les Marines
CA	Corró d'Amunt
P	Pertegàs

Annex 2

CARBON BALANCE DATA SUMMARY



NITROGEN BALANCE DATA SUMMARY



Flux ID	Calculation (units)	Data required (units) [Frequency of measure]
C1	$DQO_E\left(\frac{mg}{L}\right) \cdot Q(m3) \cdot {}^{1000L}/_{1m3} \cdot {}^{1\,Kg}/_{10^6mg} \cdot {}^{0,375KgC}/_{1KgDQO} = KgC$	$DQO_E(mg/L)$[3/S] $Q(m3)$[1/D];
C2	$DQO_S(mg/L) \cdot Q(m3) \cdot {}^{1000L}/_{1m3} \cdot {}^{1\,Kg}/_{10^6mg} \cdot {}^{0,375KgC}/_{1KgDQO} = KgC$	$DQO_S(mg/L)$[3/S] $Q(m3)$[1/D]
C3	$Q(m3) \cdot {}^{1000L}/_{1m3} \cdot (DBO_E(mg/L) - DBO_S\left(\frac{mg}{L}\right)) * {}^{1\,Kg}/_{10^6mg} * 0,7gCO2/gDBO * 0,27gC/gCO2 = KgC$	$Q(m3)$[1/D] $DBO_E(mg/L)$ [3/S] $DBO_S(mg/L)$ [3/S]
C4	$Q_{F1a}(m3) \cdot \frac{1020Kg}{m3} fang \cdot MS \cdot MSV \cdot \frac{1,42gDQO}{gSSV} \cdot {}^{0,375KgC}/_{1KgDQO} = KgC$	$Q_{F1a}(m3)$[1/D] $MS(\%)$[2/S] $MSV(\%)$[2/S]
C5	$Q_{F2a}(m3) \cdot \frac{1020Kg}{m3} fang \cdot MS \cdot MSV \cdot \frac{1,42gDQO}{gSSV} \cdot {}^{0,375KgC}/_{1KgDQO} = KgC$	$Q_{F2a}(m3)$[1/D] $MS(\%)$[2/S] $MSV(\%)$[2/S]
C6	$DQO_{CoS}(Kg) \cdot {}^{0,375KgC}/_{1KgDQO} = KgC$	$DQO_{CoS}(Kg)$[1/S]
C7	$PV = nRT;\ Q_{BioG}(m3) \cdot {}^{1000L}/_{1m3} \cdot 65\%LCH4 \cdot \frac{1}{R\left(\frac{0,082L}{atm \cdot K}\right)} \cdot \frac{P(1atm)}{T(298K)} \frac{12gC}{1molCH4} \cdot {}^{1\,Kg}/_{10^3g} = KgC$	$Q_{BioG}(m3)$[1/D]
C8	$PV = nRT;\ Q_{BioG}(m3) \cdot {}^{1000L}/_{1m3} \cdot 35\%LCO2 \cdot \frac{1}{R\left(\frac{0,082L}{atm \cdot K}\right)} \cdot \frac{P(1atm)}{T(298K)} \frac{12gC}{1molCH4} \cdot {}^{1\,Kg}/_{10^3g} = KgC$	$Q_{BioG}(m3)$[1/D]
C9	$Q_{FDesH}(Kg) \cdot MS \cdot MSV \cdot \frac{1,42gDQO}{gSSV} \cdot {}^{0,375KgC}/_{1KgDQO} = KgC$	$Q_{FDesH}(Kg)$[1/D] $MS(\%)$[2/S] $MSV(\%)$[2/S]
C10	$Q_{Centr}(m3) \cdot DQO_{Centr}\left(\frac{mg}{L}\right) \cdot {}^{1000L}/_{1m3} \cdot {}^{1\,Kg}/_{10^6mg} \cdot {}^{0,375KgC}/_{1KgDQO} = KgC$	$Q_{Centr}(m3)$[?] $DQO_{Centr}(mg/L)$[?]

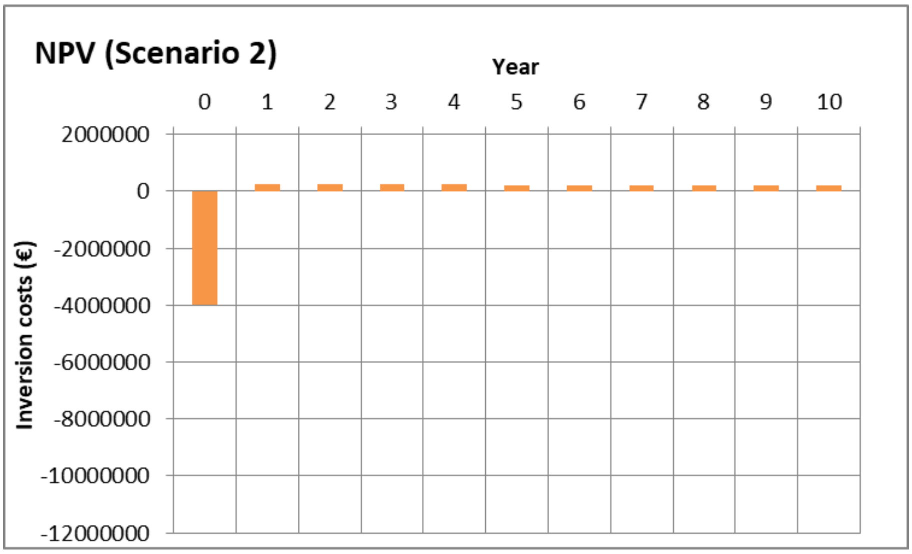
Complementary data (conversion factors): 1,42gDQO/gSSV ; 0,375gC/gDQO; 0,7gCO2/gDBO [52] 0,27gC/gCO2; 35%CO2(biogas); 65%CH4(biogas); R=0,082L/(atm·K); P=1atm i T=298K;

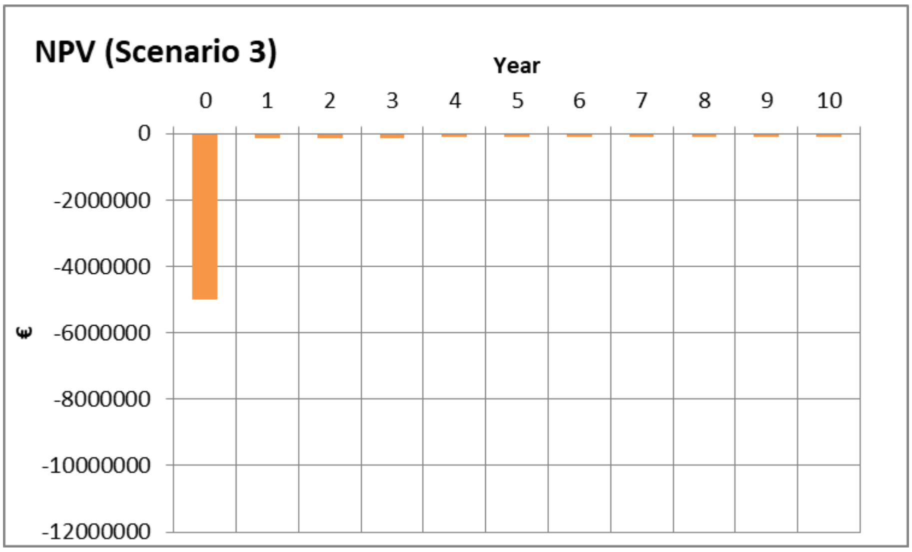
Flux ID	Calculation (units)	Data required (units) [Frequency of measure]
N1	$Nt_E\left(\frac{mg}{L}\right)\cdot Q(m3)\cdot {}^{1000L}/_{1m3}\cdot {}^{1\,Kg}/_{10^6mg} = KgN$	$Nt_E(mg/L)$[3/S] $Q(m3)$[1/D]
N2	$Nt_S(mg/L)\cdot Q(m3)\cdot {}^{1000L}/_{1m3}\cdot {}^{1\,Kg}/_{10^6mg} = KgN$	$Nt_S(mg/L)$[3/S] $Q(m3)$[1/D]
N3	$NH4_E(KgN) = KgN\ (N2)$	$NH4_E(KgN)$ [3/S]*
N4	$\left[\left(\frac{Nt_E\left(\frac{mg}{L}\right)-Nt_S\left(\frac{mg}{L}\right)}{Nt_S\left(\frac{mg}{L}\right)}\cdot 100\right)\cdot(-0{,}049)+4{,}553\right]/100\cdot N1 = KgN$	$Nt_E(mg/L)$[3/S] $Nt_S(mg/L)$[3/S]
N5	$Q_{F1a}(m3)\cdot\frac{1020Kg}{m3}fang\cdot MS\cdot MSV\cdot\frac{0{,}124gN}{gSSV} = KgN$	$Q_{F1a}(m3)$[1/D] $MS(\%)$[2/S] $MSV(\%)$[2/S]
N6	$Q_{F2a}(m3)\cdot\frac{1020Kg}{m3}fang\cdot MS\cdot MSV\cdot\frac{0{,}124gN}{gSSV} = KgN$	$Q_{F2a}(m3)$[1/D] $MS(\%)$[2/S] $MSV(\%)$[2/S]
N7	$Nt_{CoS}(Kg) = KgN$	$Nt_{CoS}(Kg)$[1/S]
N8	$Q_{FDesH}(Kg)\cdot MS\cdot MSV\cdot\frac{0{,}124gN}{gSSV}\cdot = KgP$	$Q_{FDesH}(Kg)$[1/D] $MS(\%)$[2/S] $MSV(\%)$[2/S]
N9	$Q_{Centr}(m3)\cdot Nt_{Centr}\left(\frac{mg}{L}\right)\cdot {}^{1000L}/_{1m3}\cdot {}^{1\,Kg}/_{10^6mg} = KgN$	$Q_{Centr}(m3)$[?] $Nt_{Centr}(mg/L)$[?]

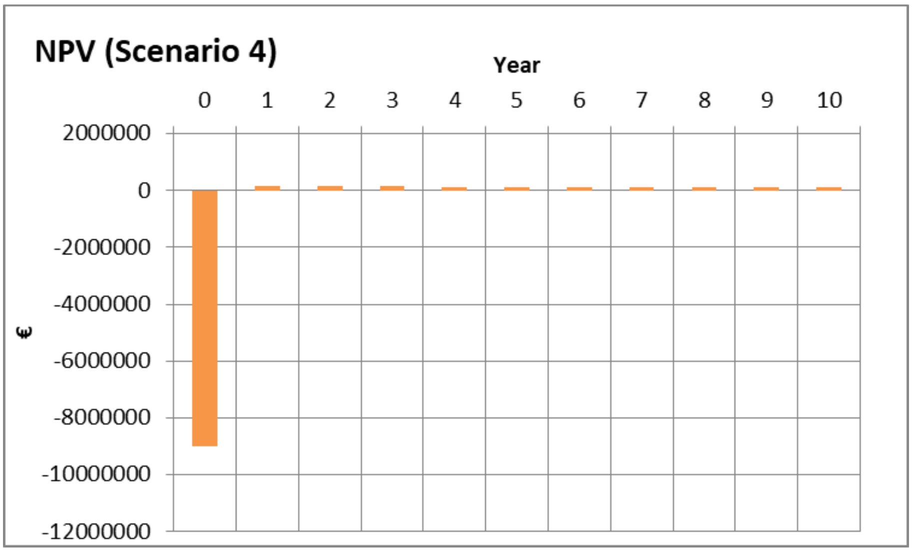
Complementary data: 0,027gp/gSSV ; Assumption of the conversion of ~100% of entering ammonia of the WWTP to N_2 (for WWTPs with nitrogen removal processes) [52]

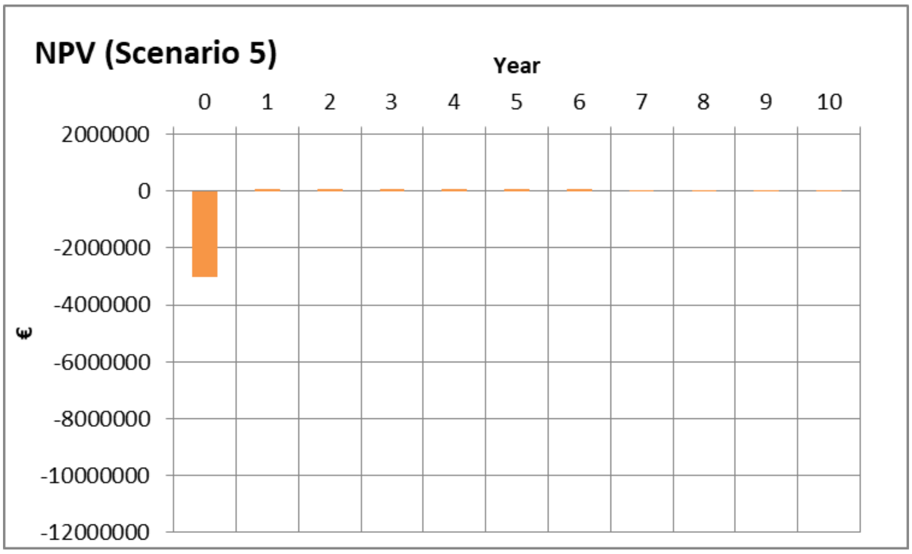
Annex 3

NPV balances








NPV (Scenario 5)
Year
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1
2
3
4
5
6
7
8
9
10
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-6000000
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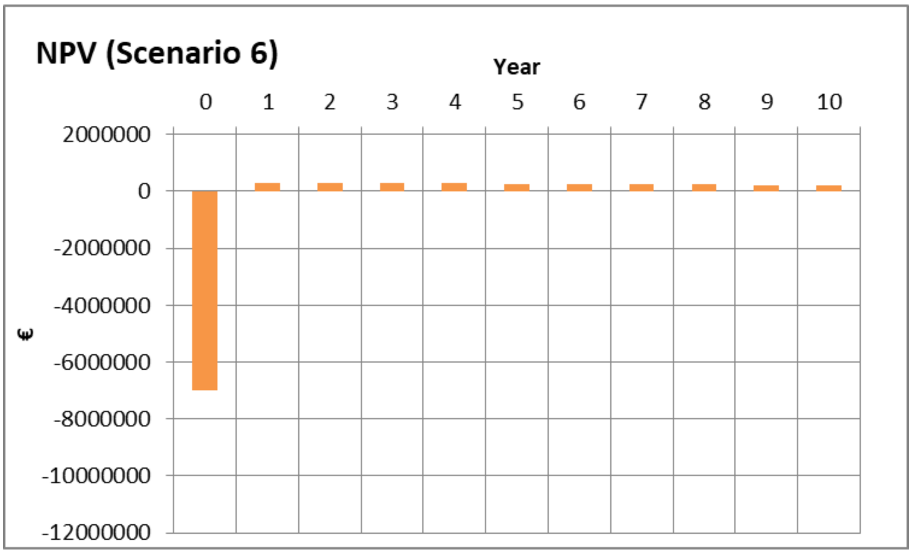
-10000000
-12000000
€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7
8
9
10
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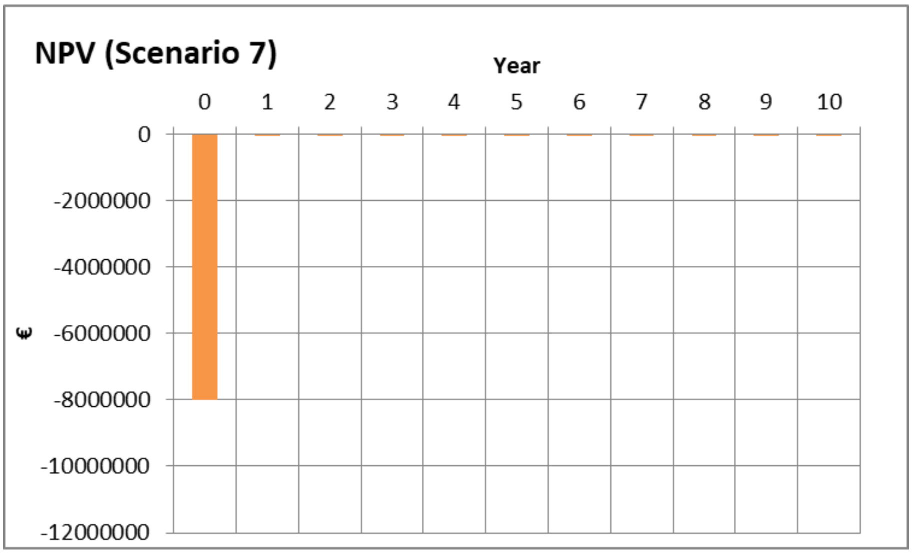
-6000000
-8000000
-10000000
-12000000
€


NPV (Scenario 7)
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8
9
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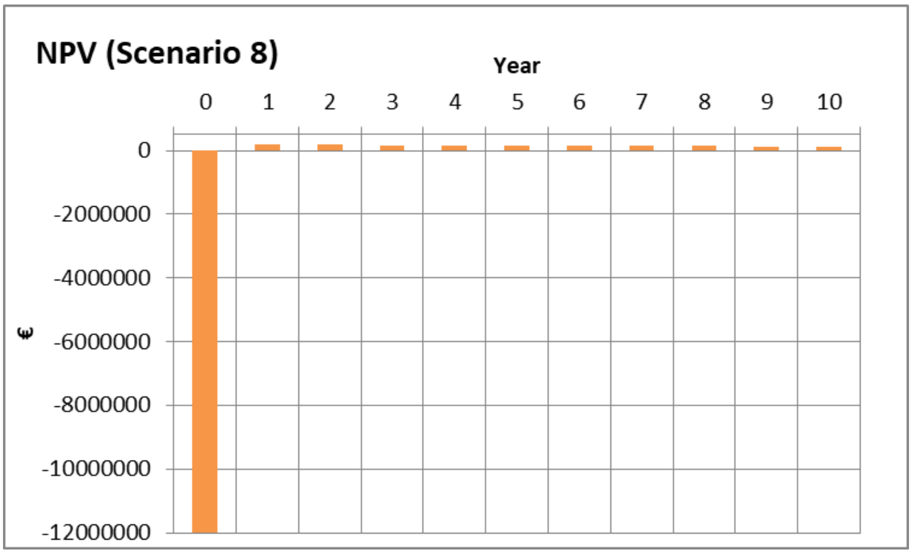
-4000000
-6000000
-8000000
-10000000
-12000000
€


NPV (Scenario 8)
Year
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3
4
5
6
7
8
9
10
0
-2000000
-4000000
-6000000
-8000000
-10000000
-12000000
€