Resource recovery from urban wastewater
-Model-based evaluation and design-

Maria-Orhideea van Schaik

Propositions

1. The success of resource recovery from urban wastewaters relies on both technology providers and product users.
   (this thesis)

2. Wastewater treatment and resource recovery models are useful only for known process performance ranges.
   (this thesis)

3. Teaching decision science mathematics at primary schools prepares youngsters for an increasingly digitalized society.

4. Promoting urban agriculture as a means to solve hunger is a fallacy.

5. The greatest challenge of innovation is implementation.

6. Children are the strongest motivation to practice science.

Propositions belonging to the thesis, entitled

Resource recovery from urban wastewater – Model-based evaluation and design

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1. Introduction

1.1 Background

1.1.1 Resource recovery

Wastewater has been considered to be a source of pollution for centuries and thus it has been collected and transported to central wastewater treatment plants (WWTPs) to be treated before being discharged into the environment. The treatment often entails energy-intensive physical, chemical, and biological processes for the removal of pollutants including organic matter, nitrogen, and phosphorus to meet local discharge regulations. However, these "pollutants", as well as the water itself, are valuable resources that can be recovered and reused. Careful and responsible recovery of resources from wastewater can contribute to the circular economy, a concept that is receiving increasing attention [1]. From a circular economy perspective, wastewater can be part of the solution for tackling energy transition, nutrient depletion, and water scarcity [2, 3, 4, 5, 6, 7].

Organic matter removal from wastewater through conventional ways (aeration and nitrification-denitrification) requires on average between 0.3 - 0.5 kWh of energy per m^3 of wastewater, mostly due to aeration [8, 9, 10]. Conventional organic matter removal results in the production of excess sewage sludge which, depending on local regulation, is most commonly applied on land, landfilled, or dewatered and incinerated [11]. Yet, organic matter contains embedded chemical energy accounting for about 1.5-2 kWh/m^3 of wastewater and can therefore be considered a source of renewable energy [8, 12]. This renewable energy source, when fully exploited, can substantially help WWTPs achieve energy self-sufficiency [10, 13, 14]. Besides contributing to energy self-sufficiency, energy recovery practices such as anaerobic digestion can also be combined with the recovery of nutrients such as nitrogen and phosphorus. These can be used either for more energy production - directly from ammonium or indirectly by producing biomass, like algae from which the energy can be retrieved [10, 7, 15, 16] - or as agricultural fertilisers [17, 18].

Nitrogen (N) and phosphorous (P) in urban wastewater are removed through processes requiring chemicals and/or energy, to avoid eutrophication in open surface water bodies. Yet both nitrogen and phosphorus can also be recovered for agricultural purposes [18]. Artificial, nitrogen-based fertilisers for agriculture, like ammonium nitrate and urea, are currently produced through extremely energy-intensive processes [19]. According to [12], the production of artificial nitrogen-based fertilisers requires between 10-15 kWh/kg N. This is comparable with the amount of energy required for the production of phosphorous-based fertilisers, requiring approximately 10 kWh/kg P. Most of the phosphorous needed for agricultural fertilisers is a depleting mineral, being mined in just a few locations and transported across the globe [20, 21, 22]. Therefore, it is subject to (worldwide) geopolitical and economic conflicts [23].

Water is also an important resource to be considered for recovery. Given the climate change scenarios, many areas on earth will experience more frequent, intense, and severe droughts [24]. Additionally, wastewater treatment and discharge requirements are becoming increasingly stringent, with micropollutants receiving increasing attention [25, 26]. Therefore, exploring possibilities for extended treatment of wastewater for reuse becomes an obvious reality [27]. In fact, wastewater is being extensively treated and reused in many parts of the world already, even as a potable water source [28, 29]. As demand for wastewater reuse is increasing, guidelines, rules and regulations for specific reuses are being formulated [30]. These are expected to support and stimulate the wider implementation of extensive wastewater treatment around the world [31].

As in some parts of the world, wastewater treatment infrastructure is aging [32, 33], has reached its maximum capacity, or in other parts is non-existent, the implementation of resource recovery becomes a real opportunity. The transition from treatment to recovery of resources from urban wastewater can become a game-changer, solving various challenges in different sectors. These challenges range from fertiliser shortage in food and non-food in agriculture to water stress in industrial, agricultural, nature conservation, and drinking water sectors.

1.1.2 Technology

Resource recovery from urban wastewater becomes even more relevant as many techniques have been and still are reaching the stage of proven reliable technologies. Technologies for energy, nutrients, and water recovery have been developed, tested, and implemented in various scenarios already for decades. Nevertheless, scenarios are not directly transferable as the success of these can strongly depend on the context defined by economic environmental, and social aspects such as affordability, legal frameworks for resource reuse, and acceptability [34, 35].

Most examples of energy and nutrient recovery are in the global north [36]. These, most commonly, stabilise, decompose, and convert the organic matter in sewage sludge into methane-rich biogas through anaerobic digestion [37, 38, 39]. This is then often converted through a combined heat and power (CHP) unit into electricity and heat [13] to power the wastewater treatment plant itself. The nutrient-rich effluent from anaerobic digestion (often referred to as digestate) is then further treated to recover phosphorus and/or nitrogen. Some processes that can be used for the direct or indirect recovery of resources from digestate include algae cultivation, crystallisation in the form of struvite or calcium phosphate, ion exchange through zeolites, membrane-based processes including forward osmosis, electrodialysis, and membrane distillation [40, 41, 42, 43, 1, 44, 45].

Recovery and reuse of water from urban wastewater mostly occurs in higher-income, freshwater-scarce countries or regions such as California and Texas in the United States, Singapore, and Australia [46, 28, 29]. The reuse of urban wastewater and the local regulation determine the required treatment [47]. For example, for urban wastewater to become potable, a complex, multi-barrier tertiary treatment is required, with intensive filtration and disinfection processes [28]. For filtration, the most common processes are sand filtration, membrane technology including micro-, ultra-, nanofiltration, reverse osmosis, and activated carbon. For disinfection, chlorination, ultraviolet treatment, ozonation, and many other (combinations of) advanced oxidation processes (AOPs) can be applied before and after filtration.

Ambitions for more efficient, cost-effective, and environmentally friendly practices, have been driving fast and diverse technology [48]. To date, hundreds of processes for wastewater treatment and resource recovery from urban wastewater and variations of these (i.e. different materials) are available on the market. Each individual process has its own characteristics which may influence the performance of a subsequent process. The performance of individual technologies however, does not give insight in the performance of combinations under varying, often context dependent, conditions [49, 50]. Therefore, treatment trains need to be evaluated as a whole to select the optimal sequence of processes and study the trade-offs made. This implies that decision-making for resource recovery is a complex task, trying to find which processes should be best used for a given wastewater and certain socio-economic contexts.

1.1.3 Decision-making

Despite all the known benefits of resource recovery (i.e. energy efficiency, water saving, income generation), there is still a lag between innovation and actual implementation of resource recovery technologies [51, 52]. This lag is a chasm and the reasons behind this are well described by the FUD factor: 'the fear, uncertainty, and doubt that can plague decision-makers when confronted with unfamiliar sets of products and services' [53]. For resource recovery from urban wastewater, the uncertainties are multi-dimensional including technical, economic, environmental, and social aspects. These uncertainties are related to the individual unit processes, the combinations of these, and/or the recovered resources themselves [54, 47, 55, 51, 56, 57, 58]. Uncertainties related to urban, regulation, and market development trends are also mentioned in the literature as important factors in implementation of resource recovery solutions [59, 60], however, these are outside the scope of the research described in this PhD thesis.

To gain more insight into and knowledge about the processes, treatment trains, and recoverable resources, decision-makers routinely choose for market research and/or pilot testing. Market research and pilot testing can, however, be time- and capital-consuming approaches [61], especially if there is already sufficient practical experience with a unit process or treatment train. Data from practical experiences can be used in a model-based approach to reproduce the multi-dimensional performance of unit processes and treatment trains [34, 62]. Such model-based evaluation and design tools can thus be used for decision support purposes as an alternative to pilot testing and market research.

1.2 Research gap

Model-based evaluation and design of treatment trains for resource recovery is challenging. While some processes or combinations of these are more efficient in removing components or are more environmentally friendly, they may hinder the recovery of resources. For example, coagulation-flocculation is efficient in removing organic matter and nutrients, however, it negatively affects the availability of organic matter for anaerobic degradation thus, lowering biogas production

[63]. Similarly, ANAMMOX is an energy-efficient process that, often used in combination with the SHARON process, removes nitrogen, offsetting it to nitrogen gas (N_2), thus disabling nitrogen recovery [64]. Moreover, when considering the recovery of multiple resources, the implementation of technology to recover one resource can affect the recovery efficiencies of another resource. For instance, the simultaneous recovery of phosphorous through, for example, struvite precipitation can affect the required nitrogen and phosphorus ratio for subsequent nitrogen recovery in the form of algae [65]. Therefore, generating treatment trains implies evaluating (i) the compatibility of processes considering the resource recovery goals and (ii) the multi-criteria performance of the sequence itself. These two aspects are equally important and should be simultaneously accounted for, as the treatment train has to fit into the local context defined by the local goals, priorities, requirements, and possibilities. While both of these aspects are individually well studied, there is a lack of understanding of how they should simultaneously be accounted for.

Existing evaluation and design frameworks and tools described in literature are fragmented, some having limited applicability and/or lacking reproducibility. Studies commonly exclude certain indicators such as social ones [66, 67] or focus only on specific ones such as environmental indicators [68, 69, 70]. Studies that simultaneously explore all impacts often focus on the recovery of a single resource [71, 72]. Some of these studies often use qualitative methods to evaluate processes and treatment trains [73] or just present their advantages and disadvantages without using clearly defined criteria and indicators [74]. Therefore, there is a lack of reproducible evaluation and design frameworks simultaneously accounting for multiple resources to be recovered and four-dimensional sustainability including technical, economic, environmental, and social aspects.

Processes for treatment and resources recovery from wastewater can perform differently depending on the reactor or unit configuration specifications (i.e. reactor shape, type and number of electrodes, membrane material and pore size), and operation conditions (i.e. hydraulic, thermal, electrical, physical, etc. conditions). However, existing tools for evaluation and design of treatment trains rely on at most minimum, maximum and average generalised performance data points per process per component removal or recovery efficiency [75, 76, 77]. Variations in process performance can be accounted for in evaluation and design tools through databases, sometimes referred to as knowledge libraries or knowledge bases or through process modelling embedded in the heuristics of a tool [78].

Knowledge libraries have the great disadvantage of becoming exponentially large and thus heavy (memory) when the number of processes increases alongside with the process performance variations. Yet, these can be managed without computational expertise. Process models, require computational skills and depending on their complexity, can become extremely computationally expensive [79, 80]. Nevertheless, simple mechanistic (white-box), semi-mechanistic (grey-box), or empirical (black-box) models can generate the necessary information for decision-making, without requiring information storage capacity [81, 82].

1.3 Research objective

As part of the NEREUS[1] Interreg 2 Seas project, this thesis aimed at establishing and exploring the building blocks of model-based evaluation and design of treatment trains for resource recovery from urban wastewater. For this, the first objective was to identify what information is needed to perform a model-based evaluation of impacts and design of treatment trains. The second objective implied the application of this information for treatment train design, evaluation, and optimisation, by developing a model able to carry out these tasks simultaneously. The third and last objective was to evaluate if grey-box process modelling can improve the model for treatment train design. With these objectives, this thesis aims to support well-informed decision-making and eventually speed up the implementation of resource recovery from urban wastewater.

1.4 Thesis outline

The aspects considered in this thesis and the focus per research chapter is presented in graphical form in Figure 1.1. An applicable set of key performance indicators (KPIs), including their definition and mathematical formulation for the design and evaluation of treatment trains (TTs) for resource recovery, is presented in Chapter 2. The KPIs are covering technical, economic, environmental, and social aspects of unit processes, the context in which these would be placed, and/or the resources that are recovered. Some of the KPIs were used in the conceptual framework of a decision support tool (DST) for designing treatment trains as presented in Chapter 4. The method applied in the DST relies on a model, which can choose compatible unit processes from a knowledge library based on a single, general performance data point per unit process. In Chapter 3 some

[1] **New Energy and Resources from Urban Sanitation** - The NEREUS project employed a decision support framework to provide evidence for different resource recovery options within various contexts. The project included pilot testing and generalized tools for evaluation and design of recovery options.

of the KPIs were also applied to compare the impacts of existing conventional wastewater treatment and new resource recovery scenarios. As an improvement to the method in the DST, the following chapters explored process modelling approaches that could be used to generate a wider range of unit process performance profiles. In Chapter 5 a grey-box modelling approach was applied to nanofiltration, a membrane process applicable for both water and nutrient recovery. This chapter aimed to evaluate how technology configuration and operation influence decision-making at the process level. The applicability of this (process modelling) approach was demonstrated through an optimisation model. Finally, an overarching discussion about the contribution and limitations of this thesis can be found in Chapter 6. In this chapter also the novelty and the missing elements with respect to simultaneous developments in the field are presented along with recommendations for future research and development.

As research continues, more technologies are emerging capable of recovering more wastewater constituents, including thermal energy, carbon compounds like cellulose and bio-polymers, and other nutrients like potassium (K), which can be recovered from wastewater [83, 84, 85, 86, 87]. Although these are not specifically covered in this thesis, they will be elaborated on in the synthesis chapter of this thesis (Chapter 6).

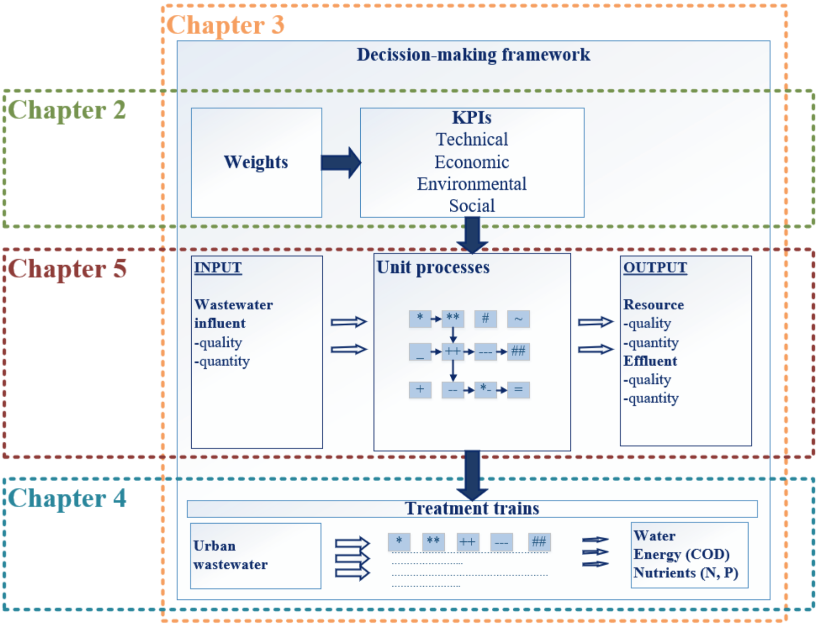

Figure 1.1: Aspects considered in the research chapters of this thesis.

2. KPIs for evaluation and design

Abstract

While urban wastewater infrastructure is aging and no longer adequate, climate change and sustainability are urging the transition from pollution management to resource recovery. Lacking evidence-based quantitative evaluation of the potential benefits and consequences of resource recovery from wastewater hinders the negotiation amongst stakeholders and slows down the transition. This study proposes mathematical formulations for technical, environmental, economic, and social key performance indicators (KPIs) that can be used to quantify the benefits and the risks of resource recovery. The proposed formulations are derived from the literature and validated with stakeholders. Each KPI is mathematically formulated at treatment train level by considering: (i) the characteristics of individual unit processes (UPs) in the treatment train (TT), (ii) the context in which the TT is installed, and (iii) the resources to be recovered. The mathematical formulations of the KPIs proposed in this study enable a transparent, consistent and informative evaluation of existing treatment trains, as well as support the (computer aided) design of new ones. This could aid the transition from urban wastewater treatment to resource recovery from urban wastewater.

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2.1 Introduction

A recent evaluation of the European Urban Waste Water Treatment Directive emphasised that compliance with the Directive requires continuous investment to replace or improve inadequate wastewater treatment plants (WWTPs) [88]. The aging of infrastructure is one of the reasons for inadequacy of WWTPs [32, 33]. Increasingly stringent regulation due to emerging pollutants and extreme weather conditions due to climate change intensify the inadequacy of conventional WWTPs [89, 7].

Wastewater can be seen as a nuisance but also as a source of reusable and valuable material [90, 91, 58]. The recovery of resources from wastewater requires a different approach towards wastewater management and treatment facility design [74, 43, 67]. An increasing number of technologies capable of recovering resources in different forms [92, 43], together with the demand for renewing aging WWTPs, provides an opportunity to renovate WWTPs towards resource recovery. To design sustainable resource recovery facilities, technical, environmental, economic, and social performance indicators need to be considered in an integrated and comprehensive way [93, 94]. However, most studies either exclude certain indicators such as social ones [66, 67] or focus only on specific ones such as environmental indicators [68, 69, 70]. Furthermore, for consistent decision-making, indicators need to represent measurable or observable quantities [95]. Relevant studies carry out a qualitative analysis which is most of the time subjective (expert-based) or when quantitative analysis is applied, the quantification method is not provided so the quantification is not reproducible. Finally, to be practically applicable, indicators should reflect the goals of stakeholders [96, 97]. However, only a few studies involved stakeholders in selecting indicators for evaluation of resource recovery from wastewater [98, 99, 100].

The transition from conventional urban wastewater treatment to resource recovery is slow, mostly because decision-makers are risk-averse and the lack of experience with novel technologies prevents them from implementing resource recovery [51]. A comprehensive quantitative evaluation of treatment facilities can provide a consistent basis for decision-making and thus speed up the implementation of resource recovery from urban wastewater [94]. Definitions and quantification of indicators used in literature are often not detailed enough to consistently evaluate technologies or treatment facilities for resource recovery and in most cases not sufficiently complete to conduct an overall integrated assessment [59, 101, 102]. Moreover, studies using various sets of indicators were often engaged in qualitative assessment, based on expert judgment [103]. Such studies do not mention which characteristics are involved and how these contribute to the assessment [78] and therefore lack in offering a rigorous scientific and reproducible approach.

Therefore, this research proposes mathematical formulations for an applicable set of key performance indicators (KPIs) to evaluate treatment facilities that recover resources. Such facilities are referred to as treatment trains (TTs) consisting of interconnected technologies represented as unit processes (UPs). The mathematical formulations are intended to support (i) model-based (computer aided) TT design, (ii) evaluation of design robustness, and (iii) decision-making. The system boundaries applied in this study and the step by step approach for KPI definition and mathematical formulations are presented in Section 2.2.1 and 2.2.2, respectively. The definitions and mathematical formulas for each KPI and their validation with the NEREUS Interreg 2 Seas project case studies are provided in Section 2.3. The study aims to support the delivery of evidence to both private and public decision-makers about the benefits of resource recovery options and help them to mitigate potential risks.

2.2 Methods

2.2.1 System boundaries

The recovery of resources from urban wastewater requires one or more interconnected unit processes (UPs) forming treatment trains (TTs) (Figure 2.1). A UP is able to treat various types of urban wastewater as well as effluents from other UPs, all varying in quality. In this study, water, total suspended solids (TSS), chemical oxygen demand (COD), total nitrogen (TN) and total phosphorous (TP) are used in mass- and flow-balances to quantify the resources recovered (water, energy, nutrients) and evaluate the achieved environmental effluent discharge requirements. Each UP entails a certain capital expenditure and uses consumables during operation and maintenance, such as energy, chemicals, replaced parts, and labour which reflect on operational expenditure.

A TT can recover a single or multiple resources. Thus, a TT can consist of several partial TTs, each individually recovering one particular resource. In case of multiple resources being recovered, the sequence of UPs recovering resource k is considered as a TT on its own (TT_k). For example, in Figure 2.1 TT_A includes UP_{X-1}, UP_X and UP_{X+1} for recovering resource A while TT_B includes UP_{X-1} and UP_Y for recovering resource B. This allows mass- and flow-balances per resource recovered and accordingly to quantify KPIs for the whole TT. A UP can serve the recovery of multiple resources (in Figure 2.1, UP_{X-1} is used to recover resource A and B), however it needs to be purchased only once.

Finally, this study focuses on KPIs that evaluate the technical, social, economic and environmental impacts of all the UPs in the TT but only within the immediate surrounding. The immediate surrounding is considered the area where the wastewater is collected, treated, discharged as well as resources recovered. The time frame considered in this study is limited to purchase and operation of UPs in the TT.

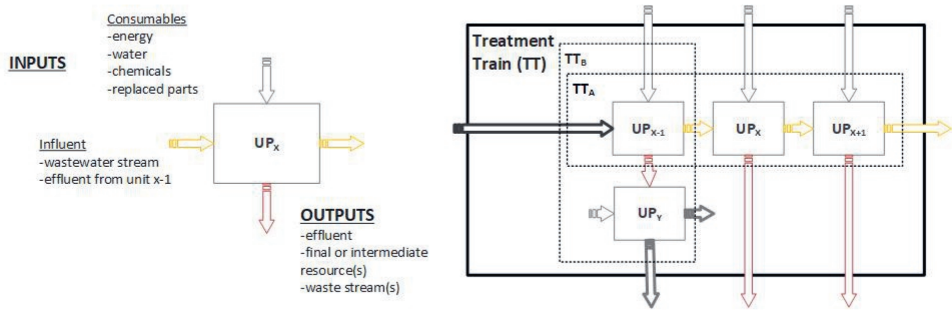

Figure 2.1: *Left: the generic representation of a unit process (UP) with the main inputs and outputs. Right: the configuration of a treatment train (TT) composed of partial treatment trains per resources (TT_A and TT_B).*

2.2.2 Defining and formulating KPIs

Various performance indicators are used in the literature on urban wastewater treatment, resource recovery from urban wastewater, and drinking water production. A brief overview of relevant studies and indicators per sustainability category (technical, social, economic and environmental) in the literature are provided in the Appendix A.2, which shows a diversity of indicators. The most common technical indicators are reliability of effluent quality, flexibility and durability (Appendix A.2, Figure A.1). Studies accounting for social indicators are mostly using acceptability and public participation (Appendix A.2, Figure A.1). Of the economic indicators, CAPEX, OPEX and net present value (NPV) are the most common ones (Appendix A.2, Figure A.2). The most chosen environmental indicators are: energy consumption and land requirement (Appendix A.2, Figure A.2). Only a few studies simultaneously account for all four categories of indicators to evaluate the recovery of water, energy and nutrients [104, 103, 105]. Overall the indicators are rarely mathematically formulated (Appendix A.2, Table A.1).

For sustainability purposes, the NEREUS project stakeholders selected from literature several key performance indicators (KPIs) for each category: technical, economic, environmental and social (Table 2.1). The stakeholders represented one government / policy-making administrative body from France; three (waste)water companies from Belgium, The Netherlands and United Kingdom; one sustainability services cooperative from Belgium; and three research institutes from Belgium, The Netherlands and United Kingdom.

Table 2.1: *Key performance indicators (KPIs) selected by the stakeholders per category: technical, environmental, economic and social.*

Technical	**Environmental**	**Economic**	**Social**
Reliability	Odour	Capital expenditure	Risk of infections
Flexibility	Noise	Operational expenditure	Risk of toxic compounds
	Footprint	Willingness to pay	Affordability
	Effluent quality	Potential income generation	Acceptability

The KPIs selected by the stakeholders were then mathematically formulated. Mathematical and phrased definitions were searched for in literature. When a KPI had already been mathematically formulated, its applicability in the given context was checked and further tailored if required. In the absence of a mathematical formulation, a formula for the KPI was generated based on phrased definitions from literature. A fill list of abbreviations for the KPIs and the parameters used in their mathematical formulations is provided in Appendix A.1. The applicability of the generated mathematical formulations was checked with the five NEREUS pilot partners. The formulations were refined based on the feedback from each pilot partner. Section 2.3.1 presents the definitions and mathematical formulations of the KPIs listed in Table 2.1. The partners were also asked to indicate what characteristics of unit processes (UPs) they could provide and thus be used to quantify the KPIs. The availability of UP characteristics per pilot partner is provided in Section 2.3.2.

2.3 Results

2.3.1 KPI definition and mathematical formulation

Economic

Capital and operational expenditure Wastewater treatment is known to involve large investments not only as capital expenditure for purchase, construction, and installation of a TT, but also as operational and maintenance expenditure [106]. Often capital expenditure (CAPEX) includes land costs [107, 108], while operation and maintenance expenditure (OPEX) includes labour costs [109]. In this study the CAPEX and OPEX of the whole TT ($CAPEX_{TT}$, $OPEX_{TT}$) are calculated as shown in Equation 2.1 and 2.2, respectively.

$$CAPEX_{TT} = \sum_{j \in TT} CAPEX_j \tag{2.1}$$

$$OPEX_{TT} = \sum_{j \in TT} OPEX_j \tag{2.2}$$

The CAPEX of a UP in the TT ($CAPEX_j$, euros) represents the one time expenditure for purchasing the UP and the OPEX is the total yearly expenditure for energy, chemicals, replaced components and required labour to operate and maintain a UP ($OPEX_j$, euros/year). When both KPIs are used at the same time, they should be expressed in the same currency.

Potential income generation Resources recovered from wastewater are reused and thus they represent reduction in $OPEX$ or a source of income [74, 55, 7]. In this study, the potential income generation (PIG) is expected to depend on the amount of resource recovered (i.e. water, nutrients, and energy) via a TT and the country-specific value of the recovered resource (adapted from [59]). The resource can be represented by a target component [50]. The target components for water, energy and nutrients are water, chemical oxygen demand (COD), and total nitrogen (TN) and total phosphorous (TP), respectively.

target component $= \{Water, COD, TN, TP\}$

The amount of recovered resources (X_k) is estimated by carrying out the mass-balance of the target component k (Equation 2.3).

$$X_k = \begin{cases} IC_k * Q_{influent} * \prod_{j \in TT_k} Y_{j,k}, & \forall k \in COD, TN, TP \\ Q_{influent} * \prod_{j \in TT_k} Y_{j,k}, & \forall k \in Water \end{cases} \tag{2.3}$$

For this, the water and mass flows of the target components need to be calculated considering the influent flow rate ($Q_{influent}$), initial concentration of each component (IC_k), and the recovery or removal percentages for water and components ($Y_{j,k}$, Equation 2.4) by each UP in TT per resource (TT_k).

$$Y_{j,k} = \begin{cases} 1 - R_{j,k} & \text{if after } UP_j \text{ target component k is in main stream} \\ R_{j,k} & \text{if after } UP_j \text{ target component k is in side stream} \end{cases} \tag{2.4}$$

where $R_{j,k}$ is the percentage of compound k that goes to the side stream in UP_j. Considering the values of the recovered products per country (VRP_{kc}), all the recovered target components need to be summed to estimate the potential income generation of the whole train (PIG_{TT}) as shown in Equation 2.5.

$$PIG_{TT} = \sum_{k \in \text{target component}} PIG_k \tag{2.5}$$

where,

$$PIG_k = X_k * H_{TT_k} * D_{TT_k} * VRP_{kc} \tag{2.6}$$

$\forall c \in country, k \in$ target component

with H_{TT_k} the number of hours of operation per day of the TT per resource k and D_{TT_k} the number of days of operation per year of the TT per resource k.

Willingness to pay According to [110], there is a threshold to the number of people willing to pay more for products and services that are associated with environmental benefits. Resource recovery from wastewater could give rise to additional $CAPEX$ and $OPEX$ thus impose higher wastewater levies on inhabitants or businesses [7]. The willingness of the population served to pay for the additional levies depends on the local economic and environmental context, as well as the costs associated with the implementation and operation of the solution [111, 112]. Thus, in this study the inhabitants' willingness to pay for environmental benefits of the whole TT (WTP_{TT}) as formulated in Equation 2.7, increases with higher net average income (NAI_c) [112], climate change awareness (CCA_c) in percentage of population served (PE), and the percentage of population served (PE) perceiving climate change as a threat (CCT_c) [111]. At the same time, the willingness to pay is likely to decrease as the costs for the TT (EAC_{TT}, Equation 2.8) increase [112].

$$WTP_{TT} = CCA_c * CCT_c * \frac{(NAI_c * PE) + PIG_{TT}}{EAC_{TT}} \tag{2.7}$$

where,

$$EAC_{TT} = \sum_{j \in TT} EAC_j \tag{2.8}$$

$$EAC_j = \frac{r(1+r)^{Lt_j}}{(1+r)^{Lt_j} - 1} * (CAPEX_j + \sum_{t=1}^{Lt_j} \frac{OPEX_j}{(1+r)^t}) \tag{2.9}$$

with r the depreciation rate in $\%$ and Lt_j the life time of a UP in years.

Technical KPIs

Reliability In the context of wastewater treatment, reliability refers to the performance of the TT (e.g. effluent quality) and can depend on the planned and unplanned maintenance activities required between potential downtime events [113, 103, 114]. Often the downtime events are caused by influent quality and quantity fluctuations [115, 116]. Thus, the lifetime, maintenance requirement and influent quality should be accounted for in comprehensive reliability evaluations of UPs. However, in this study, these will be formulated by using other KPIs, namely OPEX and flexibility, respectively.

Since wastewater treatment and resource recovery trains are series of UPs in which the performance of one UP affects the performance of the other UPs, the reliability of a whole TT (Rel_{TT}, Equation 2.10) is formulated as the product of reliabilities of all UPs (Rel_j, Equation 2.11) in the whole TT.

$$Rel_{TT} = \prod_{j \in TT} Rel_j \tag{2.10}$$

This way, the reliability of a UP is proposed to be the likelihood of the UP delivering the expected effluent or recovered resource quality. Usually, this information is provided by technology suppliers in the form of process warranty, which is a function of UP failure rate (fr_j) and for all UPs in the whole TT it should be provided for the same time frame (e.g. per year).

$$Rel_j = 1 - fr_j(p) \tag{2.11}$$

Flexibility Conventionally, in the context of (waste)water treatment, flexibility is related to (i) TT performance robustness with changing influent quality and quantity [103] but also to (ii) modularity which refers to the ease of change in the TT design configuration [117]. Since the scope of this study is to define KPIs for evaluating TTs for resource recovery from various urban wastewater streams (e.g. conventional sewage, black water, grey water, etc.), flexibility was limited to explore the optimum operating range of each individual UP [118]. Wastewater quality and quantity is typically represented by the common variables that affect the performance of UPs, i.e. concentration of TSS, COD, TN, and TP, temperature, pH and flow. Note, however, that not all UPs are sensitive to each variable. Accordingly, flexibility is estimated by normalising the min-max ranges for the variables ($range_{v,j}$, Equation 2.13) to which a specific UP is sensitive ($or_{v,j}$, Equation 2.12).

$$or_{v,j} = \begin{cases} \frac{range_{v,j}}{max_{v,j}} & \text{if } UP_j \text{ is sensitive to variable } v \\ 1 & \text{otherwise} \end{cases} \tag{2.12}$$

where,

$$range_{v,j} = max_{v,j} - min_{v,j} \tag{2.13}$$

$$\forall v \in V = \{\text{Flow, TSS, COD, TP, TN, Temperature, pH}\}$$

The final operating range per UP is the average of all normalised min-max ranges.

$$or_j = \sum_{v \in V} or_{v,j} \tag{2.14}$$

Overall, the greater the normalised min-max range, the higher the flexibility of the UP and eventually of the TT (equation 2.15).

$$Flex_{TT} = \frac{\sum_{j \in TT} or_j}{N_{TT}} \tag{2.15}$$

where, N_{TT} is the number of unit processes in the whole treatment train.

Through this KPI, model-based design and evaluation could explore the applicability of a TT with changing quality and quantity of wastewater streams.

Environmental KPIs

Odour The potential adverse effects of odours from wastewater treatment facilities on human health and environment is a critical issue that has been studied for decades [119]. According to [120], being exposed to certain odours might impact the human body in the form of anxiety, unease, headache, depression as well as some physical symptoms. Despite the developments for sampling and measuring odour, quantifying the impact of the emitted odour is not an easy task [121]. Odour emissions from wastewater treatment plants differ per process, generally decreasing from primary to tertiary treatment [101]. This can be related to the type of process (OP_j), like biological degradation of the organic matter and the status of the wastewater, like the concentration of pollutants [122].

$$OP_j = \begin{cases} 1 & \text{if } UP_j \text{ is a physical process} \\ 2 & \text{if } UP_j \text{ is a chemical process} \\ 3 & \text{if } UP_j \text{ is a biological process} \\ 4 & \text{if } UP_j \text{ is a thermal process} \end{cases} \tag{2.16}$$

The assessment of the odour emission per UP is proposed as the multiplication of the following characteristics: (i) an integer scale which indicates the odour emission potential per type of process (OP_j,) and (ii) odour emission per UP (OEP_j, Equation 2.17) based on the the maximum allowed organic matter load expressed as COD concentration ($max_{COD,j}$). If the max COD load is not available for a specific UP then the COD concentration in the UP influent ($Infl_{COD,j}$, Equation 2.18) should be taken.

$$OEP_j = \begin{cases} max_{COD,j} & \text{if max allowed COD concentration is available for } UP_j \\ Infl_{COD,j} & \text{otherwise} \end{cases} \tag{2.17}$$

where,

$$Infl_{COD,j} = \frac{IC_{COD} * Q_{influent} * \prod_{1,\ldots,j-1} Y_{j-1,COD}}{Q_{influent} * \prod_{1,\ldots,j-1} Y_{j,Water}} \tag{2.18}$$

$$Y_{j,COD} = \begin{cases} 1 - R_{j,COD} & \text{if after } UP_j\text{, COD is in the main stream} \\ R_{j,COD} & \text{if after } UP_j\text{, COD is in the side stream} \end{cases} \tag{2.19}$$

The total odour emission potential of the TT (OEP_{TT}, Equation 2.20) is estimated by summing the odour emission potentials of each UP in the TT.

$$OEP_{TT} = \sum_{j \in TT} OEP_j * OP_j \tag{2.20}$$

Noise Noise constraints for humans differ from those for animals but also per area type and time of the day [123]. According to [124] continuous noise (pressure) levels of 5-10 dB above ambient levels can affect the abundancy of some bird species. In the case of wastewater treatment plants, UPs can have a specific noise emission potential. Therefore, the levels of noise (dB) emitted by all UPs in the TT are logarithmically influencing the total level of noise (NEP_{TT}) as shown in Equation 2.21 [125].

$$NEP_{TT} = 10 * log10 \sum_{j \in TT} 10^{LNP_j/10} \tag{2.21}$$

The formulation of this KPI requires the level of noise emitted by each UP (LNP_j) in the train, expressed in dBs. Depending on the type of area in which the TT is located, sound attenuation measures have to be taken to comply with local regulation for noise emission [126].

Footprint The footprint of a WWTP indicates the surface area used for successfully achieving wastewater discharge requirements. [75] uses "land requirement" as a KPI and takes it into account in decision-making for water recovery from wastewater via a semi-quantitative measurement. According to [127] the footprint, can differ per UP, but also per type of influent stream from which resources are recovered. In this study, the footprint of a UP is evaluated via the following characteristics: (i) the area in m^2 required per m^3 of influent to be treated (A_j), (ii) the hydraulic retention time (HRT_j), and (iii) the influent flow rate ($Q_{influent}$). The sum of footprints of all UPs in the TT is then used to estimate the footprint of the whole train as presented in Equation 2.22.

$$FP_{TT} = \sum_{j \in TT} A_j * HRT_j * Q_{influent} \tag{2.22}$$

Effluent quality Effluent quality is the main indicator for monitoring the performance of a wastewater treatment plant. Conventionally, wastewater treatment plants are operated such that the final effluent quality complies with local discharge regulations. Effluent discharge regulations differ per country and are stated per pollutant. Pollutant removal efficiencies per UP ($R_{j,i}$) are used to predict final effluent quality by evaluating the achieved final concentration of pollutants in the main stream ($FC_{i,water}$, Equation 2.23).

$$FC_{i,water} = \frac{IC_i * \prod_{j \in TT_{Water}} (1 - R_{j,i})}{\prod_{j \in TT_{Water}} (1 - R_{j,Water})} \tag{2.23}$$

where,

$$\forall i \in Pollutants = \{TSS, COD, TN, TP\}$$

The total removal of each pollutant needs to comply with legal requirements for different discharge locations such as open surface water body, designed surface water body, existing sewer. Depending on the effluent quality standards to be met, a compliance index per TT, in the main stream ($EQCI_{TT}$) is calculated via a pollution index as presented in Equation 2.24.

$$EQCI_{TT} = \begin{cases} 1 & \text{if } PI_{TT_{water}} = 0 \text{ (complying with legislation)} \\ 0 & \text{if } PI_{TT_{water}} \geq 1 \text{ (not complying with legislation)} \end{cases} \tag{2.24}$$

The pollution index ($PI_{TT_{water}}$, Equation 2.25) is estimated for the main stream (adapted from [102]) by summation of the pollution index per pollutant (PI_i, Equation 2.26).

$$PI_{TT_{water}} = \sum_{i \in Pollutants} PI_i \tag{2.25}$$

For this, the limit concentrations of pollutants (legal requirements) for different discharge locations ($LC_{i,l,water,c}$) need to be compared with the final concentrations of pollutants in the main stream ($FC_{i,water}$).

$$PI_i = \begin{cases} 1 & \text{if } LC_{i,l,Water,c} < FC_{i,Water} \\ 0 & \text{otherwise} \end{cases} \tag{2.26}$$

where,
i $\in$ $Pollutants$, l $\in$ discharge location, c $\in$ countries.

Social KPIs

Risk of toxic compounds Hazard free recovered resources are dependent on the efficiency of TTs in removing potentially toxic compounds present in the original influent such as heavy metals, dyes, other trace organic compounds, etc. [128]. Similarly to the pollution index proposed by [102], this study proposes a ratio ($RatioToxic_{tc,TT_k}$, Equation 2.27) between the limit concentrations ($LC_{tc,k,c}$) determined by regulations [129, 130, 131, 30, 132, 28] and the predicted final concentration ($FC_{tc,k}$, Equation 2.28) to evaluate the contamination of recovered resources with any toxic compound.

$$RatioToxic_{tc,TT_k} = \frac{FC_{tc,k}}{LC_{tc,k}} \tag{2.27}$$

$$\forall tc \in \text{toxic compound and} \qquad \forall k = \{Water, TN, TP\}$$

where,

$$FC_{tc,k} = \begin{cases} \frac{IC_{tc} * \prod_{j \in TT_k} Y_{j,tc}}{\prod_{j \in TT_k} (Y_{j,Water})} & k : \{TN, TP\} \\ IC_{tc} * \prod_{j \in TT_k} Y_{j,tc} & k : \{Water\} \end{cases} \tag{2.28}$$

$$Y_{j,tc} = \begin{cases} 1 - R_{j,tc} & \text{if after } UP_j\text{, toxic compound tc is in main stream} \\ R_{j,tc} & \text{if after } UP_j\text{, toxic compound tc is in side stream} \end{cases} \tag{2.29}$$

If any of the toxic compounds in any of the recovered resources in the whole TT exceeds the maximum allowed concentration then there is a risk of contamination with toxic compounds. Otherwise, the higher the $RatioToxic_{tc,TT_k}$ the lower the risk of toxic compounds (RTC_{TT}, Equation 2.30).

$$RTC_{TT} = \begin{cases} 0 & \text{if any } RatioToxic_{tc,TT_k} \leq 1 \text{, no risk} \\ 1 & \text{if any } RatioToxic_{tc,TT_k} > 1 \text{, potential risk} \end{cases} \tag{2.30}$$

Risk of infection The risk of infection is a great concern when water and nutrients are being recovered from wastewater and reused. The WHO has established a calculation method for this based on the degree of exposure, severity and duration of diseases, as well as the number of people affected [28]. This KPI is proposed as a binary indicator to check whether the potential risk of infection is present per resource to be recovered based on the predicted pathogen removal and the removal requirements. The removal of pathogens by UPs is generally expressed in log reductions and the total removal of a specific pathogen (TLR_{i,TT_k}, Equation 2.31) is the sum of the log reductions ($LR_{i,j}$) of all UPs in the TT.

$$TLR_{i,TT_k} = \sum_{j \in TT_k} LR_{i,j} \forall i \in pathogen \tag{2.31}$$

where,

$$\forall i \in \text{ pathogen and} \qquad \forall k : \{Water, TN, TP\}$$

The required pathogen removal is also expressed in log reduction and represents the ratio between the concentration of the pathogen in the influent and the regulatory (health-based) standard per recovered resource ($Cpe_{i,k}$[2]) that could be nationally or internationally valid [129, 130, 131, 133, 30, 28].

$$RLR_{i,k} = log10 \frac{IC_i}{Cpe_{i,k}} \tag{2.32}$$

Finally the risk of infection potential (ROI_{TT}) is calculated via the ratio between required log reduction ($RLR_{i,k}$, Equation 2.32) and the total log reduction achieved by a TT per resource (TLR_{i,TT_k}, Equation 2.31) as shown in Equation 2.33.

[2]Limit concentration of pathogen i equivalent to 10^{-6} DALYS pppy for resource k.

$$ROI_{TT} = \begin{cases} 0 & \text{if any } \frac{RLR_{i,k}}{TLR_{i,TT_k}} \leq 1, \text{ no risk} \\ 1 & \text{if any } \frac{RLR_{i,k}}{TLR_{i,TT_k}} > 1, \text{ potential risk} \end{cases} \tag{2.33}$$

Acceptability This indicator is expected to heavily depend on the need for the recovered resources. Therefore, acceptability of the resources recovered from wastewater by the society might show differences based on the following: (i) the shortage of the product in the country or region [134], (ii) degree of human contact, and (iii) potential perceived risks [135].

The shortage of the resource is proposed as the demand-supply ratio of this resource per country [136]. The degree of human contact (HC_k) depends on the specific use of the resources, such as water for agriculture [131], food industry [30] or irrigation of parks, and non-edible gardens [134].

$$HC_k = \begin{cases} 1 & \text{if k is energy} \\ 2 & \text{if k is nutrients} \\ 3 & \text{if k is irrigation water} \\ 4 & \text{if k is industrial water} \\ 5 & \text{if k is drinking water} \end{cases} \tag{2.34}$$

The potential perceived risk ($RatioInfection_{TT_k}$, Equation 2.35; $RatioToxic_{TT_k}$, Equation 2.36) is evaluated via the achieved removal rate of pathogens (TLR_{i,TT_k}) and toxic compounds ($FC_{tc,k}$).

$$RatioInfection_{TT_k} = \sum_{i \in pathogen} \frac{RLR_{i,k}}{TLR_{i,TT_k}} \tag{2.35}$$

$$RatioToxic_{TT_k} = \sum_{tc \in \text{toxic compounds}} \frac{FC_{tc,k}}{LC_{tc,k}} \tag{2.36}$$

The KPI formulation as proposed in this study (Equation 2.37) shows that the higher the demand-supply ratio ($DS_{k,c}$) and the lower the degree of human contact (HC_k) with resource in consideration, the more acceptable a TT is.

$$Acceptability_{TT} = \sum_k \frac{DS_{kc}}{RatioInfection_{TT_k} * RatioToxic_{TT_k} * HC_k} \quad (2.37)$$

where,

$k \in$ recovered resources, $c = country$

Affordability Affordability is intrinsically context dependent [101] and generally considered to be an economic indicator [137]. For example, in low-income countries affordability and simplicity play an important role while in high-income countries, sustainability is one of the most commonly used and aimed for concepts [138]. In this study affordability is considered to be a social KPI, indicating the purchasing power of a community. The mathematical formulation proposed for this KPIs is provided in Equation 2.38.

$$Affordability_{TT} = \frac{(PE * NAI_c) + PIG_{TT}}{EAC_{TT}} \quad (2.38)$$

With this method it is assumed that the higher the population size served by the TT and the net average income, the more affordable a TT becomes. The characteristics that are expected to negatively affect affordability are equivalent annual costs (EAC_{TT}, Equation 2.8), as these would increase the levies that the population served has to pay. The affordability would however increase when capital income is expected from the sales of the recovered resources (PIG_{TT}, Equation 2.5).

2.3.2 Case studies

The applicability check revealed that a few UP characteristics are not available for all the UPs tested by the NEREUS pilot partners (Table 2.2 based on Table A.2 and A.3 from Appendix A.3). For example, the level of noise emission per UP is not readily available. Unless the UP suppliers can provide this information or the noise levels are measured, it will not be possible to quantify this environmental KPI as proposed in this study. Similarly, the removal percentage of certain toxic compounds as well as the removal of specific pathogens are not available for all UPs. Therefore, the risk of toxic compounds and the risk of infection cannot be calculated. The calculation of these two KPIs can also be affected by the inconsistency between the available data on removal percentages of specific compounds and the limit concentrations for these compounds. For example, there is a

Table 2.2: *Applicability check with pilot partners (PP) of the NEREUS project. + means that data per characteristic needed to calculate the specific KPI is fully available; +/- means that data per characteristic needed to calculate the specific KPI is not available for all UPs in the TT; - means that data per characteristic needed to calculate the specific KPI is not available for any of the UPs in the TT.*

Criteria	KPI	PP 1	PP 2	PP 3	PP 4	PP 5
Economic	Capital expenditure	+	+	+	+	+
	Operational expenditure	+	+	+	+	+
	Potential income generation	+	+	+	+	+
	Willigness to pay	+	+	+	+	+
Technical	Reliability	+	+	+	+	+
	Flexibility	+	+	+	+	+
Environmental	Odor	+	+	+	+	+
	Noise	+/-	+/-	+/-	+/-	+/-
	Footprint	+	+	+	+	+
	Effluent quality	+	+	+	+	+
Social	Risk of toxic components	-	+	-	+	-
	Risk of infection	-	-	-	-	-
	Acceptability	+	+	+	+	+
	Affordability	+	+	+	+	+

limit concentration for E.coli in fertilising products. The removal percentages of this pathogen are known for some UPs such as anaerobic digestion but they are neither known nor measured for other UPs such as sieves and electro-coagulation. Moreover, the concentrations of specific toxic compounds and pathogens in the influent should be provided as well to determine their fate in the treatment train. At the time of the validation, only pilot partner 1 and 4 could provide influent concentrations for a chosen heavy metal (i.e. Pb), while none of the partners could provide the influent concentrations of pathogens (i.e. E. coli).

2.4 Discussion

This study proposes an applicable set of KPIs, including their definition and mathematical formulation for the design and evaluation of treatment trains (TTs) for resource recovery. Each KPI is mathematically formulated by considering the characteristics of (i) individual unit processes (UPs), (ii) the context in which they are installed, and (iii) the resources to be recovered. This study succeeded in mathematically formulating the KPIs such that they can be applied for any TT, context, and resource(s) to be recovered.

While mathematically formulating KPIs, in this study two categories were observed: (i) constraints (go/no go) and (ii) evaluation indicators. The first category, constraints are indicators that use legislative or regulative characteristics in their definition. These set the limitations to which a TT is environmentally and socially viable [51] and thus which TT may be considered for further evaluation. From Table 2.1 the following KPIs are constraints: effluent quality (EQCI, Equation 2.24), risk of toxic compounds (RTC, Equation 2.30), risk of infections (ROI, Equation 2.33).

Overall, resource recovery and reuse related risks can be of various kinds including human health, environment, management, and financial. Risk of infection and risk of toxic compounds are the two most important risks related to the reuse of recovered resources [51], addressing human health and safety. Affordability, acceptability, willingness to pay (WTP) and the potential income generation (PIG) are other KPIs proposed in this study that could be used to evaluate financial and management related risks.

During the definition and formulation process, overlaps between KPIs were acknowledged. The value tree approach (Figure 2.2) was used to visualise the overlaps of the UP characteristics used in the formulation of each KPI [139]. Some UP characteristics were used in the formulation of more than one KPI. Accordingly, the more often a characteristic is used the higher the importance of that characteristic in the final evaluation. Furthermore, it can be observed that eventually all categories of KPIs make use of removal/recovery percentages of effluent quality parameters, showing that the same parameters are used to evaluate seemingly different aspects. While acceptability and affordability could be evaluated via social inquiries, in this study the evaluation was broken down to UP level to differentiate quantitatively between treatment alternatives.

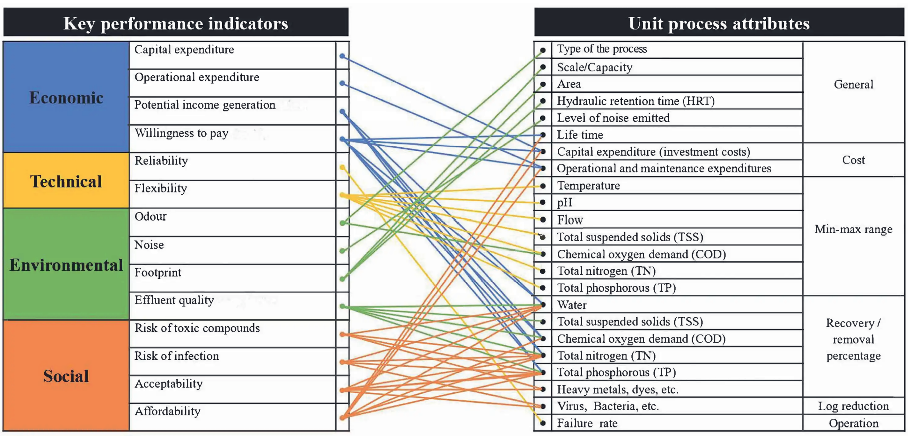

Figure 2.2: *Unit process characteristics (right) used in the mathematical formulation of key performance indicators (left).*

Several KPIs were defined by using other KPIs considered in this study. For example, affordability and willingness to pay (WTP) were formulated with the help of the following economic KPIs: CAPEX, OPEX and potential income generation (PIG). Since the recovery/removal percentages of UPs are needed to calculate the PIG, these UP characteristics are eventually used in the formulation of PIG, affordability, and WTP. While the mathematical formulas of these three KPIs clearly overlap, their meaning is essentially different. Each individual KPI has its own meaning and thus should be considered for TT evaluation and design purposes.

The validation of the mathematical formulations revealed that the quantification of KPIs can be affected by the lack of data per UP. The lack of data per UP can be explained in two ways: (i) the data is not needed or considered irrelevant or (ii) the data is not available. This leaves two options to the end-user or decision-maker: (i) the KPI is considered irrelevant or (ii) the KPI is important and data should be collected for current and future use.

By providing a clear definition with mathematical formulation for KPIs, this study creates a transparent interface whereby the decision-maker or end-user gains insight into the content of each KPI. Firstly, the KPIs can be used to evaluate the contribution of individual UPs and accordingly to assess the impact of replacing technology for adaptation of the treatment facility towards future needs. Secondly, the KPIs can be used to evaluate the robustness of a planned design when for example influent characteristics and product quality requirements change. Thirdly, the KPIs allow the user to study trade-offs between various technologies and assign weights to show the importance of each KPI, resulting in balanced and consistent decision or design evaluation. Uncertainties related to the mathematical formulations of the KPIs will be incorporated into a future study by means of sensitivity analysis.

2.5 Conclusions

Mathematically formulating a set of sustainability KPIs as proposed in this study enables a transparent and consistent evaluation of existing TTs and supports the (computer aided) design of new solutions. The KPIs provide insight into the selection of alternative technologies and trade-offs during design and decision-making, and they indicate to what extent certain social, technical, environmental and economic aspects influence the evaluation of a treatment facility. For design purposes social and environmental constraints are critical, since they ensure viability of the TT. Mathematically formulating these constraints contributes to understanding the importance of aligning information from technology suppliers with local, national or international regulation.

3. Model-based design - conceptual framework

Abstract

In the context of circular economy, wastewater can be used to address some of the 21st century's challenges regarding the transition to renewable resources for water, energy, and nutrients. Despite all the research, development, and experience with resource recovery from urban wastewater, its implementation is still limited. The transition from treatment to resource recovery is complex due to the difficulty of selecting unit processes from a large number of candidate processes considering the operational limitations of each process, and sustainability objectives. Presently, a multi-criteria decision support tool that deals with the difficulty of unit process selection for resource recovery from wastewater has not been developed. Therefore, this paper presents the conceptual framework of a decision support tool to find the optimum treatment train consisting of compatible unit processes which can recover water, energy and/or nutrients from a specified influent composition. The framework presents the relationship between the user input, the knowledge library of technologies and a weighted multi-objective nonlinear programming model to aid process selection. The model presented here shows, not only how the processes are selected, but also the four-dimensional sustainability impact of the generated treatment train while considering the weight provided by the user. Thus, this study presents a reproducible framework which can support private and public decision-makers in transparent evidence-based decision making and eventually the systematic implementation of resource recovery from urban wastewater.

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3.1 Introduction

With the current water use patterns and population growth rates by 2030 the global water demand for different purposes including drinking, irrigation, and industry is expected to be 60% higher than the global water supply, this even without taking into consideration the climate change-related water stress [140, 141]. This will be accompanied by a proportional increase in wastewater generation [142]. According to [143] more than 4% of the global electricity consumption is used for the extraction, treatment and distribution of water and wastewater and the water consumption is projected to double by 2040. Regarding nutrients present in wastewaters, it is estimated that 16.6 million tonnes of nitrogen (N) and 3 million tonnes of phosphorus (P), representing 13 % of the global demand for agriculture, are discharged annually into the global sewerage network causing widespread eutrophication of receiving water bodies [43, 144]. At the same time the growing global population has increased the demand for food and nutrient rich fertilisers (N and P) much of which is secured from unsustainable sources. This juxtaposition stresses the need for resource recovery from urban wastewater which can significantly contribute to the circular economy [145] by converting wastewater into valuable sources of energy and clean water, as well as nutrients [146, 147].

To unlock the benefits of resource recovery from urban wastewaters four- dimensional sustainability (i.e. economical, technical, environmental, and social) has to be considered in the design of resource recovery facilities [104, 78, 148]. Resource recovery facilities are treatment trains, consisting of a sequence of unit processes that treat wastewater to the required compliance standard and recover resources. Treatment trains are system engineering and design products, in which (i) the performance of a discreet unit process can affect the performance of the whole treatment train and (ii) the performance of the treatment train can also be affected by short or long term influent quality and quantity changes [149]. Therefore, in this study, the conventional triple bottom line approach for sustainability was extended to a four-dimensional sustainability by considering also technical indicators.

Generating optimal treatment trains is challenging due to: (i) the vast number of available unit processes, (ii) the variability of wastewater influents in quantity and quality with time and location, (iii) multiple targeted resources, (iv) the influence a selected unit process has on the downstream processes, and (v) having multi-dimensional sustainability goals. The decision-making process becomes even more complicated when considering regulatory requirements which depend on the geographical and social context [150, 151]. Selecting and combining unit processes to effectively recover resources from urban wastewater is thus complex and traditionally has been based on labour intensive, trial-and-error experiments and expert judgement [152]. Decision support tools (DST) can assist decision-makers to deal with these complexities. Presently, Novedar EDSS [78], WiSDOM [35], Poseidon [75], MOSTWATAR [153] are examples of DSTs in the field of wastewater treatment and water recovery and reuse. However, existing tools do not generate treatment trains by simultaneously encompassing:

- multi-resource recovery (water, energy, nutrients, etc.) from urban wastewater
- different resource quality levels
- country specific regulations and requirements
- four-dimensional sustainability
- criteria and indicators weighting

Thus, a DST that shows the potential of resource recovery through evaluating the synergies and trade-offs between the different sustainability dimensions is needed.

In response to the limitations of existing tools, this study proposes a conceptual framework for the NEREUS-DST to recommend a treatment train to recover water (drinking, irrigation and industrial water), energy (chemical energy) and/or nutrients (nitrogen and/or phosphorus) from a specified urban wastewater. The recommendation is based on local regulations, priorities and the trade-offs between sustainability dimensions, considering economic, environmental, social and technical aspects. The NEREUS-DST is part of the NEREUS Interreg 2 Seas project which aims to support public and private decision-makers with the decision-making process and eventually accelerate the implementation of resource recovery from urban wastewater. The DST aims to enables public and private decision-makers to evaluate the impacts of different recovery options and thus identify which resource is best to recover at a given location. Moreover, the policy makers and technology suppliers could use this framework to harmonise over standards for resource reuse purposes and the knowledge required for decision-making.

This conceptual framework presents the main building blocks of the web-based NEREUS DST: user input, knowledge library, multi-criteria decision-making process and output. The multi-criteria decision-making process consists of a weighted multi-objective mixed integer nonlinear programming (WMOMINLP) model for the selection of optimum unit processes considering the four sustainability dimensions. To solve the WMOMINLP model, an exact solution method is used: the Branch-And-Reduce Optimisation Navigator (BARON) via GAMS Optimisation-Solver solver [154]. With this level of transparency, this study aims to enable the academia to identify the areas that can be further developed such that the decisions concerning resource recovery from wastewater can be made more accurate and objective, and thus more suitable for specific contexts.

This paper is organised in 5 sections. In Section 3.2, an overview of existing decision support tools used in wastewater treatment and reuse is provided. Section 3.3 presents the methodology describing (i) the conceptual framework of the NEREUS DST and (ii) case study used for demonstration purposes. In Section 3.4, the results of the case study are presented and discussed. Finally, concluding remarks are made and suggestions for further research are proposed in Section 3.5.

3.2 Overview of DSTs for (waste)water treatment and resource recovery

Over the past 20 years, DSTs became increasingly relevant to wastewater treatment as they can provide scenario-based evidence on the performance and impact of treatment trains, but the evidence is often limited to only some specific evaluation criteria. After searching for decision support tools and decision support systems for (waste)water treatment and resource recovery in the academic literature, the authors identified and reviewed 23 relevant studies (Table 3.1). The search was conducted until December 2020, without limiting the search to a specific time period, using search engines such as Scopus, Science Direct, and Google Scholar. The aim of the review was to find existing design-based tools or systems to generate treatment trains for resource recovery from urban wastewater. The reviewed studies present both selection- and design-based prototype or fully developed computer-based decision support tools or systems, providing the connection between the main building blocks of a DST: user input, database and outputs. Studies that only present and apply selection-based (multi-criteria) decision-making approaches, without showing the building blocks of a DST and the connection between these blocks, were excluded from the review.

Researchers developed computerised decision support systems for the design of wastewater treatment plants in the 1990s, mostly taking into account technical objectives in order to comply with discharge regulation and economic aspects to inform decision makers about financial consequences related to the regulations [155, 156, 157, 158]. Only more recently the social and environmental aspects have been accounted for in the decision-making processes [159]. This has been largely driven by the onset of climate change and increasing global population. Currently social and environmental indicators turn out to play a critical role in ensuring viability of new wastewater and resource recovery treatment train designs as described in detail by [149]. Therefore, future DSTs should be capable of managing the complexity of technologies, while supporting decision-makers to create a positive socio-economic value, to protect the environment and thereby human health [160].

Table 3.1: *Overview of DSTs in (waste)water treatment and resource recovery literature.*

DST Name	**Sustainability Dimensions**	**Context**	**Method**	**Purpose**	**Ref.**
(prototype)	Techno-economic	WWT	Mathematical techniques	Design	[156]
(prototype)	Techno-economic	WWT	Expert system fuzzy logic	Design	[157]
SOWAT	Techno-economic	WWT	Heuristic ANP with Fuzzy sets	Design	[155]
MEMFES	Techno-economic, Environmental	Membrane-based treatment systems for metal finishing	AHP	Design	[158]
SANEX	Economic, Social	Selection of sanitation systems	Multi-attribute utility theory	Evaluation	[161]
(no name)	Economic	IWWT sequence generation	Knowledge-based Heuristic	Design	[162]
(no name)	Techno-economic	Drainage water treatment and reuse	Static knowledge-base	Design	[163]
MOSTWATAR	Techno-economic, Environmental, Social	Water reuse	Genetic Algorithm	Design	[153]
WAWTTAR	Economic	WWT and Water Reuse	Modelling simulation	Evaluation	[164]
WASDA	Technical	IWWT and Municipal WWT	technical process design	Design	[165]
WADO	Economic	Industrial process water systems	Heuristic MINLP	Design	[166]
WTRNet	Techno-economic, Environmental	Water reuse with Network distribution	Combined simulation model with MILP	Design	[108]

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DST Name	Sustainability Dimensions	Context	Method	Purpose	Ref.
MEDAWARE	Economic, Environmental, Social	Existing wastewater facilities	Relational database for multi-criteria	Evaluation	[167]
WASWARPLAMO	Techno-economic, Environmental, Social	Feasibility assessment for water reuse	Ranking	Evaluation	[168]
(prototype)	Economic, Environmental, Social	Wastewater management solutions	Ranking	Evaluation	[169]
ROUTES	Techno-economic, Environmental	Sludge processing and disposal	Integrated assessment	Evaluation	[170]
NOVEDAR EDSS	Techno-economic, Environmental, Social	WWT	Decision Tree AHP	Design	[78]
FitWater	Techno-economic, Environmental, Social	WWT	Fuzzy weighted average method	Evaluation	[171]
IDST	Techno-economic, Environmental	Treatment trains for unconventional water supplies	MOO	Design	[172, 173]
IRIPT	Techno-economic, Environmental, Social	Satellite WWT	PROMETHEE	Evaluation	[174]
Wisdom	Techno-economic, Environmental	WWT	NSGAII	Design	[35]
Poseidon	Techno-economic, Environmental	Water reuse	MCDA	Design	[75]
(prototype)	Techno-economic, Environmental, Social	WWT	N/A	Design	[175]
NEREUS (Conceptual Framework)	Technical, Economic, Environmental, Social	Multiple Resource Recovery	MINLP	Design	This study

ANP: Analytic Network Process, AHP: Analytic Hierarchy Process, MCDA: Multi-criteria Decision Analysis , MI(N)LP: Mixed Integer (Non) Linear Programming, MOO: Multi-Objective Optimisation, NSGAII: Non-Dominated Sorting Genetic Algorithm, PROMETHEE: Preference Ranking Organisation METHod for Enrichment of Evaluations, WWT: Wastewater Treatment, IWWT: Industrial Wastewater Treatment

In addition to the evaluation criteria, existing DSTs also vary depending on (i) the context for which they were developed, (ii) the embedded method and (iii) the purpose of the tool (Table 3.1). DSTs have been developed for a wide range of contexts, including municipal and industrial wastewater treatment [165, 166], general wastewater management including network distribution [108], sludge processing [170] and water reuse [168]. However none of the existing DSTs aims to generate trains for the recovery of water, energy and/or nutrients at the same time.

Most DSTs in the literature employ various multi-criteria decision-making methods (MCDM) for evaluating a pre-defined set of alternative solutions (Table 3.1). MCDM methods such as multi-attribute utility theory, ranking, fuzzy weighted average method and PROMETHEE are used to identify the best solution from the set of alternatives [161, 171, 174]. These methods are selection-based, depending on the pre-defined solution alternatives. Design-based decision-making methods on the other hand explore the full set of solution alternatives. However, the number of DSTs that generate solutions by using multi-objective optimisation (MOO) methods is relatively limited (3 of the 23 reviewed studies in Table 3.1) and these methods have not previously been applied to generate solutions for multi-resource recovery from urban wastewater.

The current paper explored the application of MOO methods for multi-resource recovery by presenting and implementing a conceptual framework to generate treatment trains that can simultaneously recover water, energy and/or nutrients from urban wastewater. The framework makes use of the MOO method to balance out economic, environmental, social and technical aspects represented by several indicators.

3.3 Methodology

The methodological approach of this study consists of (i) presenting the main building blocks of the NEREUS DST conceptual framework and (ii) demonstrating the framework through two hypothetical cases representing small and large wastewater treatment plants. The case study approach tests the applicability of the presented framework. Nine scenarios around the two cases (Table 3.7) are used to show and discuss the responsiveness of the framework on the criteria weighting and targeted resources.

3.3.1 Conceptual Framework of web-based NEREUS DST

The conceptual framework of the NEREUS DST defines the information required and how it is processed in order to (1) find an optimal treatment train, (2) estimate resource recovery efficiencies and final concentrations of components, and (3) appraise four-dimensional sustainability performance. The key building-blocks of the NEREUS DST are the user input, a knowledge library, the multi-criteria decision-making process and the DST output. The content of the building-blocks and the interactions between them are presented in Figure 3.1 and detailed in the following subsections.

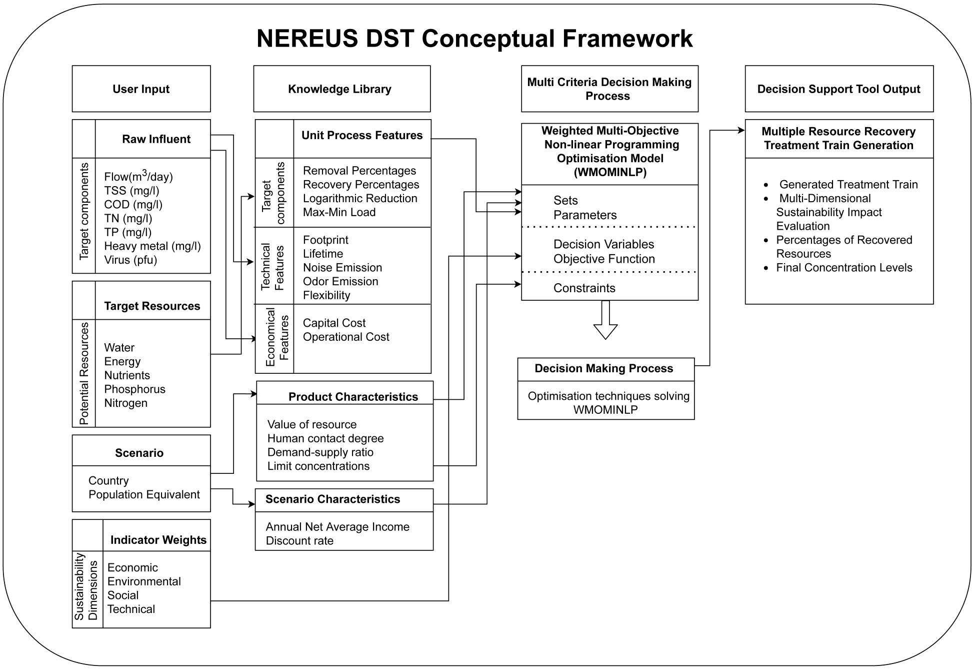

Figure 3.1: *The conceptual framework of the NEREUS DST.*

User input

The output of the DST is dependent on the information that the DST user provides as input. The DST requires the user to: (i) provide raw influent quality and quantity characteristics; (ii) choose the target resources to be recovered; (iii) select the country in which the treatment train would have to be installed; and (iv) provide weights for the sustainability dimensions and their indicators.

The raw influent characteristics for the selection of unit processes currently are: total suspended solids (TSS), chemical oxygen demand (COD), total nitrogen (TN), total phosphorus (TP), heavy metals (HM) and viral load. The targeted resources for recovery in the NEREUS DST are listed under three main categories including (i) the type of water (drinking, irrigation, industry, discharge) , (ii) energy represented by COD [176], and (iii) nutrients represented by TN and/or TP. The DST users can then choose to recover water for a specific purpose including drinking, irrigation, and industrial. However, when the user chooses to recover only energy or nutrients the model generates a treatment train to ensure the effluent to meet site-specific effluent discharge reg ulations. In this study, to be consistent across several countries and simultaneously represent recoverable resources, the following effluent q uality p arameters h ave b een c hosen: TSS, COD, TN, and TP. Since discharge and recovered resource reuse regulations vary by country, the user must select the country that the treatment train will be installed. Currently, the legislative requirements of The Netherlands, Belgium, France and the United Kingdom are included.

Different decision-makers have different priorities and objectives when optimising for sustainability. The novelty of this DST is the four-dimensional sustainability impact evaluation which is systematically assessed based on the specific features of the unit processes and user input. The DST assesses the impacts of unit processes and treatment trains by using indicators in each dimension: economic, environmental, social and technical. The DST then collects the weights for both the main dimensions and the indicators. These weights account for the relative importance in decision-making, while reflecting the priorities of the user. The importance of each indicator is set by the user setting the weight in a hierarchical approach. In this approach, first the weights of the main dimensions are set by the users with the total weight adding to 100%. Then, the weights of the indicators within each dimension should be set such that they add up to 100%. This demonstrates that, by collecting and setting the weights, the DST can provide tailored outputs to the user.

Knowledge library

The knowledge library contains a database with, (i) the features of the relevant unit processes, (ii) effluent discharge and recovered resource quality regulation, and (iii) country specific information. This database is needed in the multi-criteria decision-making process that explores treatment train alternatives.

The list of unit processes and their capital and operational expenditures, removal and recovery percentages for specific c omponents, a nd t he r ange o f permitted influent (min-max) concentration levels are included in the database. This information helps to build the connection between legal requirements and performance efficiency of the treatment train generated. Finally, the recovered resources reuse regulations should also be known. The stored information is also used in the evaluation of sustainability dimension.

In this study, the conceptual framework incorporates the fundamental components of the knowledge library required for decision-making in the given context. A knowledge library was created and made available for testing the current version of the tool through the hypothetical cases. This knowledge library can and will be extended and made available to the users, as the DST will be further developed.

Multi-criteria decision making process: Weighted Multi-Objective Mixed Integer Nonlinear Programming Model

The NEREUS DST embeds a multi-criteria decision-making process that utilises the user input and the knowledge library to generate a treatment train. This treatment train consists of a series of unit processes that can treat a specific wastewater (influent) and recover the desired resource(s), while fulfilling the four-dimensional sustainability goals. A schematic process flow diagram of a treatment train, showing a general sequence of unit processes, the streams - both main and side -, and the specific resources that can be recovered from each stream are presented in Figure 3.2.

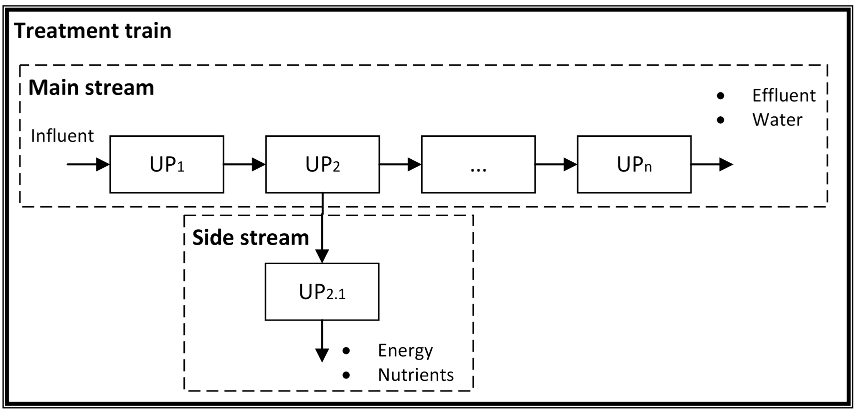

Figure 3.2: *A general process flow diagram of a treatment train consisting of unit processes (UP_i).*

To facilitate multi-criteria decision-making, a weighted multi-objective mixed integer non-linear programming (WMOMINLP) model is proposed in this study. The model ensures that the unit processes in the treatment train can operate together to meet regulatory requirements and recover resources. The proposed conceptual optimisation model consists of the following components: (1) sets, (2) parameters, (3) decision variables, (4) the objective function, and (5) constraints as explained in the next subsections. The content of these components is presented in the next sections and is highly dependent on the key performance indicators per sustainability dimension. In this study only a few of the key performance indicators presented by [149] were used to demonstrate and implement the conceptual framework.

Sets used in WMOMINLP model

The sets represent the problem dimensionality and ensure compactness and flexibility of the optimisation model. In this way, the elements in the set can be added and removed based on the needs of the modeller. The sets used in the proposed WMOMINLP model are listed in Table 3.2. In the model, set UP includes the unit processes that are subject to the selection of a treatment train that can recover resources EP. Depending on their features and functionality, unit processes can carry out tasks that include: energy recovery, phosphorus recovery, nitrogen recovery and water disinfection. These tasks are represented by set T. Considering the set of tasks, set UP is divided into two subsets. The subsets represent the unit processes that can operate in the main stream $UP_{T,Main}$ or in the side stream $UP_{T,Side}$. The unit processes in the main stream can contribute to the recovery of water. Unit processes treating the side streams are better suited for the recovery of resources such as energy or nutrients but not water since COD, TN, and TP are more concentrated in the side stream. Furthermore, considering the features of the unit processes in the knowledge library, set UP is divided into four subsets: UP_{Group1}, UP_{Group2}, UP_{Group3}, UP_{Group4}. These subsets include unit processes with similar minimum required and maximum allowed influent COD (chemical oxygen demand) concentration levels, to ensure unit processes are ordered in a logical treatment flowsheet. In this optimisation model a list of components presented as set C is used for quantifying the recovered resources as well as the concentration of unwanted components in specific streams. The sustainability dimensions are represented in set D. As mentioned in Section 3.3.1, the sustainability dimensions are evaluated through indicators. The quantification of these indicators is based on the descriptions and mathematical formulations from [149]. These indicators for each sustainability dimension (economic, environmental, social and technical) are represented in set I_D.

Table 3.2: *Sets of the WMOMINLP model.*

Sets	Description	Elements
T	The set of tasks that can be carried out by unit processes	Energy Recovery, Phosphorus Recovery, Nitrogen Recovery, Water Disinfection
EP	The set of potential resources that can be recovered by a treatment train	Drinking Water, Irrigation Water, Industrial Water, Energy, N-fertiliser, P-fertiliser
WEP	The set of water qualities that can be recovered	Drinking Water, Irrigation Water, Industrial Water
UP	The set of unit processes that are subject to selection	
Subset UP		
	$UP_{T,Main}$	The set of unit processes that can perform task $t \in T$ in main stream
	$UP_{T,Side}$	The set of unit processes that can perform task $t \in T$ in side stream
	UP_{Group_1}	The subset of UP with minimum COD concentration level of 600 mg/l
	UP_{Group_2}	The subset of UP with maximum COD concentration level of 600 mg/l
	UP_{Group_3}	The subset of UP with maximum COD concentration level of 100 mg/l
	UP_{Group_4}	The subset of UP with maximum COD concentration level of 40 mg/l
C	The set of components used for calculation of concentration levels and amount of recovered resources	Water, TSS, COD, TN, TP, Virus Load, Heavy Metal
D	The set of four-dimensional sustainability dimensions	Economic, Environmental, Social, Technical
I_D	The set of indicators per sustainability dimensions	I_{Econ} : PIG, EAC I_{Env} : $OD, dB, Land$ I_{Soc} : $Acceptability, Affordability$ I_{Tec} : $Flex$

PIG: Potential Income generation, EAC: Equivalent Annual Cost, OD: Odour, dB: Noise, $Land$: Land Requirement, $Flex$: Flexibility

Table 3.3: *Parameters of the WMOMINLP model.*

Unit process features	
$P_{c,i}$	The removal percentage of component $c \in C$ by unit process $i \in UP$ (%)
$RP_{c,i}$	The potential recovery percentage of component $c \in C$ by unit process $i \in UP$ (%)
LR_i	The log reduction of unit process $i \in UP$ (log)
$Capex_i$	The capital expenditure of unit process $i \in UP$ (€)
$Opex_i$	The operational expenditure of unit process $i \in UP$ (€)
A_i	Surface area required unit process $i \in UP$ (m^2)
LT_i	Expected lifetime of unit process $i \in UP$ (years)
LNP_i	The noise potential level of unit process $i \in UP$ (dB)
O_i	The odour emission level of the unit process $i \in UP$ in a scale of 0-3 (n.d.)
FL_i	The flexibility level of unit process $i \in UP$ in a scale of 1-10 (n.d.)
C	The set of components used for calculation of concentration levels (n.d.)
Product characteristics	
r	The yearly discount rate (%)
PE	The size of population that the treatment train is intended to serve (p.e.)
NAI	The annual net average income of the country where the treatment train will be implemented (€/year)
$Target$	The resources that are targeted to be recovered and selected by the user (n.d.)
$NTarget$	The nutrient resources that are targeted to be recovered and selected by the user (n.d.)
$WTarget$	The water resources that are targeted to be recovered and selected by the user (n.d.)
W_D	The weighting of the sustainability dimension $d \in D$ between 0 and 1 (n.d.)
$W_{s,d}$	The weighting of the indicator $s \in I_D$ and $d \in D$ between 0 and 1 (n.d.)
Target values	
$Z^*_{s,d}$	Target value of sustainability indicator $s \in I_D$ and $d \in D$ for scaling (NA)

n.d.=non-dimensional; p.e.=population equivalent; NA=not applicable

Parameters used in WMOMINLP model

Parameters represent prior knowledge either provided by the user or embedded in the knowledge library. The parameters are coefficients that are used with decision variables to build the constraints and can also be used for what-if scenario and sensitivity analysis. Table 3.3 presents the parameters used in the model under three main categories: (1) features of unit processes, (2) user input and (3) characteristics of resources to be recovered. An additional (intermediate) parameter is required to store the target values representing the best possible performance for each indicator. The target values are calculated by solving the model as a single objective per indicator prior to multi-objective optimisation. These values help to scale the indicators used in the calculation of the overall objective function.

Decision Variables used in WMOMINLP model

The decision variables in mathematical programming indicate a set of values that need to be determined in order to solve the problem. When the model is solved using optimisation methods, the best (optimum) values of the decision variables are found. In this WMOMINLP model, the decision variables determine the unit process selection (x_i) and the sustainability indicator values ($Z_{s,d}$). Variable x_i is a binary variable depending on whether unit process i is selected ($x_i = 1$) or not ($x_i = 0$). The sustainability indicators and auxiliary decision variables are formulated using x_i and various parameters. The auxiliary decision variables are part of the evaluation of the indicators. The full list of variables to be determined by solving the model is provided in Table 3.4.

Table 3.4: *Decision Variables of the WMOMINLP model.*

Decision variables	
x_i	The binary variable depending on whether unit process $i \in UP$ is selected ($x_i = 1$) or not ($x_i = 0$) (n.d.)
$Z_{s,d}$	The decision variable representing the sustainability indicators where $s \in I_d$ and $d \in D$
$Z_{EAC,Econ}$	Equivalent annual cost of the treatment train (€/year)
$Z_{PIG,Econ}$	The potential income generation by the recovered resources(€/year)
$Z_{Acceptability,Soc}$	The acceptability of the recovered products based on treatment train (n.d.)
$Z_{Affordability,Soc}$	The affordability of the treatment train based on the selected unit processes (n.d.)
$Z_{Land,Env}$	The land area required for the treatment train (m^2)
$Z_{OD,Env}$	The odour level in the treatment train (n.d.)
$Z_{dB,Env}$	The noise emission level of treatment train (dB)
$Z_{Flex,Tech}$	The flexibility of the treatment train (n.d.)
Auxiliary decision variables	
R_c	The amount of recovered component $c \in C$ through the treatment train (m^3;kg)
TLR	The total log removal of viruses in the treatment train (log)
$RiskRatio_k$	The indicator of risk level based on the ratio between the reached level of toxic compounds, pathogens and the required (regulated) levels for the product k (n.d.)

n.d.=non-dimensional; p.e.=population equivalent; NA=not applicable

Objective function used in WMOMINLP model

A multi-objective optimisation model often has multiple conflicting objectives and aims to balance the trade-off between these objectives. The objective function of the WMOMINLP model aims to minimise the weighted sum of the normalised difference between values $Z^*_{s,d}$ and $Z_{s,d} \forall s \in I_d, \forall d \in D$ simultaneously. The best possible value per indicator, stated in parameters as target value $Z^*_{s,d}$, is determined by optimising one objective at a time. Subsequently, these values are used as a normalisation factor. Specifying the importance of sustainability dimensions is a key consideration for the selection of unit processes. Therefore, to consider the user's priority for each sustainability dimension, the proposed model includes the weights for both main dimensions (W_d) and their indicators ($W_{s,d}$). The objective function of the model is stated in Equation 3.1 .

$$minimise \sum_{s,d \in I_d, d \in D} W_{s,d}.W_d.\frac{|Z_{s,d} - Z^*_{s,d}|}{Z^*_{s,d}} \tag{3.1}$$

Constraints used in WMOMINLP model

Constraints define the possible values the decision variables of the WMOMINLP model may take. The constraints that enable the generation of feasible treatment trains are formulated and shown in Table 3.5. In the same way, the equations that calculate the value of the decision variables for the sustainability impacts are also presented in Table 3.5. The decision variables are calculated in a similar fashion as the constraints, with mathematical equalities and inequalities, and are therefore also implemented in the DST accordingly.

Equations 2-9 represent the four-dimensional sustainability impacts of the treatment train. The mass of recovered components is calculated through the equations 10-13, where COD, TN, TP and water represent the recovered resources: energy, N-fertiliser, P-fertiliser and water, respectively. The indicator of risk is based on the ratio between the reached removal of toxic compounds (HM), pathogens ($Viral\ load$) and the maximum allowed (regulated) levels of HM and $Viral\ load$ per product k are represented in equations 14-15 for water and nutrients. Depending on the targeted water quality, the equations 16-18 ensure the total logarithmic reduction of viruses reached by the selected unit processes is greater than the regulatory requirements.

Depending on the targeted resource to be recovered, constraint 19 ensures that at least one unit process is selected to recover nitrogen and phosphorus either for main stream or side stream. Similarly, constraint 20 ensures that only one unit process which can recover energy is selected for the main or the side stream. Constraints 21 - 23 ensure that the influent is compatible with the unit processes from specific groups. This way the model prevents the selection of incompatible unit processes. Constraint 24 ensures that the quality of recovered water or effluent complies with the regulations for all the compounds in set C. Similarly, depending on the targeted nutrient and the required quality, constraint 25 ensures that the concentration level of heavy metals in the recovered resource is lower than values provided in EU directives for the use of N and P as a fertiliser. Additionally, constraints 26 to 29 represent the sign constraints regarding the decision variables. The framework components explained in this section are demonstrated with a case study in Section 3.4.

Table 3.5: *Constraints of the WMOMINLP model.*

Constraint formula	**Equation**
Sustainability indicator	
$Z_{EAC,Econ} = \sum_{i \in UP} (r.(1+r)^{Lt_i})/((1+r)^{Lt_i}-1).(CAPEX_i + \sum_{t=1}^{Lt_i}(OPEX_i)/((1+r)^t)).x_i$	(3.2)
$Z_{Flex,Tech} = \frac{\sum_{i \in UP} Flex_i x_i}{\sum_{i \in UP} x_i}$	(3.3)
$Z_{Land,Env} = 1.15.\sum_{i \in UP} A_i.x_i$	(3.4)
$Z_{Acceptability,Soc} = \frac{\sum_{k \in Target} DS_{k,l}}{RiskRatio_k * HC_k}; l \in Country$	(3.5)
$Z_{Affordability,Soc} = \frac{(PE.NAI_l)+Z_{PIG}}{Z_{EAC}}; l \in Country$	(3.6)
$Z_{OD,Env} = \sum_{i \in UP} O_i.x_i$	(3.7)
$Z_{dB,Env} = 10.log10(\sum_{i \in UP} x_i.10^{\frac{LNP_i}{10}})$	(3.8)
$Z_{PIG,Eco} = \sum_{k \in Target} R_k.365.VRP_k$	(3.9)
Mass of recovered component	
$R_{COD} = M_{COD}.(1 - \prod_{i \in UP_t}(1 - (RP_{COD,i}.P_{COD,i}.x_i)).(\sum_{i \in UP_{Side,Energy}}(RP_{COD,i}.P_{COD,i}.x_i) + \sum_{i \in UP_{Energy,Main}}(RP_{COD,i}.P_{COD,i}.x_i)); t \in Group1, Group2$	(3.10)

continued on the next page

Constraint formula	Equation
Mass of recovered component	
$R_{TN} = M_{TN}.(1 - \prod_{i \in UP_t}(1-(RP_{TN,i}.P_{TN,i}.x_i))). \prod_{i \in UP_{Side,Nitrogen}}(1-((1-RP_{TN,i}.P_{TN,i}).x_i));$ $t \in Group1, Group2, Group3, (Nitrogen, Main)$	(3.11)
$R_{TP} = M_{TP}.(1 - \prod_{i \in UP_t}(1-(RP_{TP,i}.P_{TP,i}.x_i))). \prod_{i \in UP_{Side,Phosphorus}}(1-((1-RP_{TP,i}.P_{TP,i}).x_i));$ $t \in Group1, Group2, Group3, (Phosphorus, Main)$	(3.12)
$R_{Water} = Q. \prod_{i \in UP_{t,Main}}(1-(1-P_{water,i}.x_i)); t \in T$	(3.13)
Risk level	
$RiskRatio_{Water} = RLR/TLR$	(3.14)
$RiskRatio_k = \frac{R_k}{Purity_N.M_{HM}.(1-(i \in UP_{t,Main}(1-(P_{HM,i}.x_i)))).10^6}$; $\forall k \in NTarget$ and $t \in T$	(3.15)
Log reduction	
$TLR \geq RLR$	(3.16)
$RLR = log_{10}(Inf_{Virus} - Directive_{Virus})$	(3.17)
$TLR = \sum_{i \in UP} LR_i.x_i$	(3.18)
Ensuring UP selection	
$\sum_{i \in UP_{t,Main}} x_i + \sum_{i \in UP_{t,Side}} x_i \geq 1 \forall t \in NutrientRecovery$	(3.19)
$\sum_{i \in UP_{t,Main}} x_i + \sum_{i \in UP_{t,Side}} x_i = 1 \forall t \in EnergyRecovery$	(3.20)
Influent compatibility with the group	
$\frac{M_{COD} \prod_{i \in UP_t} 1-(P_{COD,i} * x_i)}{Q * \prod_{i \in UP_t} 1-((1-P_{Water,i}).x_i)} \leq 600; t \in Group1$	(3.21)

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Constraint formula	Equation
Influent compatibility with the group	
$\frac{M_{COD} \prod_{i \in UP_t} 1-(P_{COD,i} * x_i)}{Q * \prod_{i \in UP_t} 1-((1-P_{Water,i}).x_i)} \leq 100; t \in Group1, Group2$	(3.22)
$\frac{M_{COD} \prod_{i \in UP_t} 1-(P_{COD,i} * x_i)}{Q * \prod_{i \in UP_t} 1-((1-P_{Water,i}).x_i)} \leq 40; t \in Group1, Group2, Group3$	(3.23)
Recovered water compliance	
$\frac{M_c \prod_{i \in UP_{t,Main}} 1-(P_{c,i} * x_i)}{R_{Water}} \leq Directive_{c,WTarget}; t \in UP_{Main}$	(3.24)
Recovered resource compliance	
$\frac{R_k}{M_{HM}(1- \prod_{i \in UP_{t,Main}} (1-P_{HM,i} x_i)} \leq Purity_k.Directive_k.10^6; \forall k \in NTarget$	(3.25)
Sign constraints	
$x_i \in \{0,1\}; \forall i \in UP$	(3.26)
$R_c \geq 0; \forall c \in C$	(3.27)
$Riskratio_k \geq 0; \forall k \in Target$	(3.28)
$Z_{s,d} \geq 0; \forall s \in I_d$ **and** $d \in D$	(3.29)

3.3.2 Case study description

In this section, two hypothetical UK cases representing small and large scale wastewater treatment plants (WWTPs) were used to test the application of the NEREUS DST framework. A typical large and small WWTP were selected to investigate the tool's response to different scales. The influent quality and quantity specifications for these two hypothetical cases are provided in Table 3.6.

Table 3.6: *The influent characteristics of two UK cases.*

Parameter	**Flow rate**	**Population equivalent**	**TSS**	**COD**	**TP**	**TN**	**Lead**	**Viruses**
Unit	m^3/day	-	mg/l	mg/l	mg/l	mg/l	mg/l	pfu/100ml
Case 1	100 000	400 000	464	193	6.6	60	0.1	1 000 000
Case 2	3 500	20 000	500	300	11	44	0.1	1 000 000

The responsiveness of the model to (i) changing weights per sustainability dimension and (ii) targeted resource recovery was tested through eight scenarios developed around case 1. One scenario represents the conventional approach to wastewater treatment without resource recovery. For this scenario, the weighted multi-objective MINLP model is solved to find a treatment train that meets the effluent discharge requirements. A ninth scenario is developed around case 2 to compare different scales, aiming to recover the same resources and using the same weights as the first scenario of case 1. The scale, targeted resources and the weights for the scenarios are provided in Table 3.7.

The knowledge library, used in the case study, includes 31 different unit processes with features collected from Poseidon DST [75] and the Noverdar DST [78]. The regulatory requirements for recovered resources and effluent discharge were based on the European directives [177, 178, 179, 180, 28]. Similarly, the commercial values of the recovered resources represent the average prices for the European market. An approximate value for the treated wastewater, lower than the commercial values of the recovered water, is used to represent the avoided pollution levies and potentially required capital and operational expenditures to make sure the plant complies with regulation [181].

Table 3.7: *The nine scenarios developed around the two UK cases.*

Case	Scenario	Scale	Targeted resources	Weights
Case 1	ENPD-EW	Large	Energy (E); Nitrogen (N); Phosphorus (P); Drinking Water (D)	Equal weighting, 25% each
	ENPD-ECN	Large	Energy (E); Nitrogen (N); Phosphorus (P); Drinking Water (D)	100% economic
	ENPD-SOC	Large	Energy (E); Nitrogen (N);Phosphorus (P); Drinking Water (D)	100% social
	ENPD-ENV	Large	Energy (E); Nitrogen (N); Phosphorus (P); Drinking Water (D)	100% environmental
	ENPD-TEC	Large	Energy (E); Nitrogen (N); Phosphorus (P); Drinking Water (D)	%100 technical
	ENPI-EW	Large	Energy (E); Nitrogen (N); Phosphorus (P); Irrigation Water (IW)	Equal weighting, 25% each
	ED-EW	Large	Energy (E); Drinking Water (D)	Equal weighting, 25% each
	DIS-EW	Large	Discharge (DIS)	Equal weighting, 25% each
Case 2	S-ENPD-EW	Small	Energy (E); Nitrogen (N); Phosphorus (P); Drinking Water (D)	Equal weighting, %25 each

3.4 Results and discussion

To generate treatment trains for the scenarios defined in Section 3.3.2, the proposed WMOMINLP model is implemented and solved by using GAMS Optimisation - Solver (GAMS Development Corporation, 2011). The Branch-And-Reduce Optimisation Navigator (BARON) solver, which can be used for the global solution of nonlinear (NLP) and mixed-integer nonlinear programs (MINLP), is used as a global optimal solution method. The NEOS server [182] is used to run the scenarios and the computational time did not exceed 3 seconds for all scenarios. The selected unit processes per scenario are presented in Section 3.4.1 and the associated impacts and amount of resources recovered are presented in Section 3.4.2.

3.4.1 Selected unit processes

From the 31 unit processes in the knowledge library, 24 were selected in total for the nine scenarios with the selected unit processes for each scenario (Table 3.8). The number of unit processes selected for the scenarios aimed to achieve drinking water quality ranged between 9 and 10. For the scenario recovering irrigation water instead of drinking water (ENPI-EW) and the scenario treating water for discharge (DIS-EW), the model selected only 6 and 4 unit processes, respectively. Thus, the more stringent the recovered resource quality parameters, the greater the chance that more unit processes are needed. Each selected unit process has a specific impact on sustainability dimensions: economic, social, environmental and technical. The cumulative impacts of selected unit processes for each scenario are presented and discussed based on the sustainability dimension in Section 3.4.2. The validity of model output depends on the quality and quantity of the information provided by the user, and available in the knowledge library. The more accurate the information provided by the user is, the more tailored the output of the model will be. The accuracy of the model output can be limited by the amount of information available in the knowledge library [183]. The current library is only used for evaluation purposes in this paper.

The model does not (yet) provide the exact location of unit processes within a group in the treatment train and thus the model approximates the resource recovery percentages (Figure 3.5). To provide the exact location of unit processes, heuristics with a lot of logic ('if-then') rules from experts are required [76]. However this would increase the reliance of decision-making on the expert judgement but also limits the flexibility of the model and thus the number of solution alternatives [184]. Based on the grouping approach explained in Section 3.3.1, the best order of the unit processes selected by the model can be decided and the percentages can be recalculated. As an example, the potential sequence of the selected unit processes for scenario ENPD-EW and the recalculated recovery percentages as well as the waste streams (in grey) are presented in Figure 3.3. It is important to note that the inventory and further treatment of the solid waste streams are outside the scope of this study.

Table 3.8: *The selected unit processes per scenario.*

Groups	Unit processes	Case 1 - Large ENPD-EW	ENPD-ECN	ENPD-SOC	ENPD-ENV	ENPD-TEC	ENPI-EW	ED-EW	DIS-EW	Case 2 - Small S-ENPD-EW
Group 1	Sedimentation without coagulant							X		
	Sedimentation with coagulant	X	X	X	X		X		X	
	Flocculator + Clarifier					X				X
Group 2	Activated sludge	X					X	X	X	
	Low loaded AS with denitrif. + SS					X				
	Trickling filter with SS		X	X						
	Membrane bioreactor									
Group 3	Dual media filter	X	X	X	X	X	X	X		X
	Microfiltration	X	X		X			X		X
	Ultrafiltration			X					X	
Group 4	Nanofiltration	X	X	X	X	X		X		X
	Reverse osmosis	X		X	X	X		X		X
	Activated carbon		X							
	Ion exchange	X	X	X	X			X	X	X
Group 5	Advanced oxidation process	X	X	X	X	X		X		X
	Electrodialysis					X				
	Ozonation					X				
	Chlorine dioxide					X	X			
Group 6	Anaerobic digestion					X				
	UASB				X					
	EGSB									X
	Pyrolysis	X	X	X			X	X		
Group 7	Struvite Precipitation	X	X	X	X	X	X			X
	Stripping		X							

AS: activated sludge; SS: secondary sedimentation; ENPD: energy, nitrogen, phosphorous, and drinking water recovery; ENPI: energy, nitrogen, phosphorous, and irrigation water recovery; ED: energy and drinkingwater recovery; DIS: discharge water quality; EW: equal weighting; ECN: 100% economic; SOC: 100% social; ENV:100% environmental; TEC: 100% technical; S: small scale

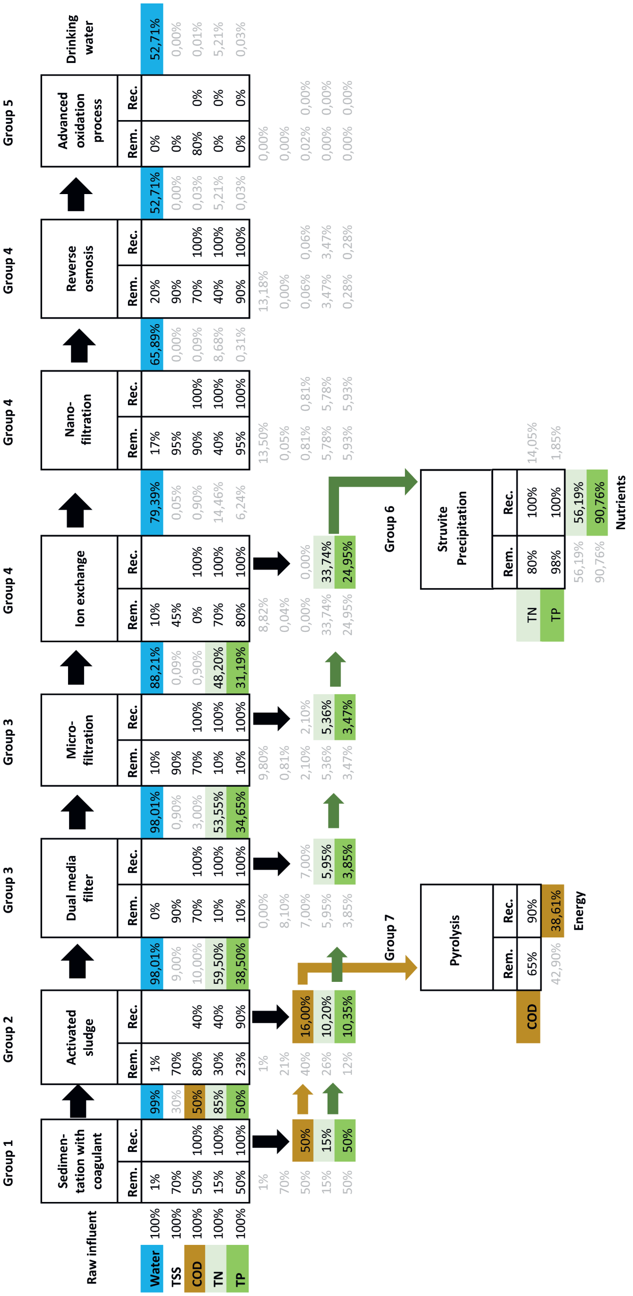

Figure 3.3: *Potential order of the selected unit processes for ENPD-EW. Highlighted in blue, light green, dark green, brown are the recovery percentages of water, nitrogen, phosphorus, and COD, respectively.*

3.4.2 Sustainability dimensions and performance indicators

The model selects unit processes to recover the targeted resources while balancing the trade-off between the prioritised dimension via the associated weights. The sustainability dimension impact and the approximated resource recovery percentages per scenario are presented in Figure 3.4 and Figure 3.5. Based on these results, some basic evaluations and comparisons can be made with the current model.

Scenarios	Economic		Environmental			Social		Technical
	EAC	PIG	Noise	Odor	Land requirement	Affordability	Acceptability	Flexibility
	M €/year	M €/year	dB	-	ha	-	-	-
ENPD-EW	53.5	27.1	24.5	3	21.8	15.4	3.3	6.2
ENPD-ECN	51.9	33.1	25.1	7	23.2	16.0	3.2	5.6
ENPD-SOC	52.1	25.6	24.6	4	23.0	15.8	3.3	5.9
ENPD-ENV	268.3	27.8	24.2	3	7.6	3.1	3.2	6.0
ENPD-TEC	72.6	29.5	24.6	8	36.5	11.4	3.0	7.1
ENPI-EW	9.6	27.2	22.3	4	20.9	85.9	2.2	6.8
ED-EW	52.6	25.1	23.6	3	21.9	15.6	1.4	6.3
DIS-EW	15.2	1.3	19.9	3	1.0	52.3	0.1	6.0
S-ENPD-EW	4.9	0.9	23.8	4	0.4	8.3	3.0	6.4

Figure 3.4: *The impacts of the sustainability indicators per scenario.*

Scenarios	Recovery COD	Recovery TN	Recovery TP	Recovery Water
ENPD-EW	39%	66%	92%	53%
ENPD-ECN	32%	64%	90%	66%
ENPD-SOC	32%	64%	90%	50%
ENPD-ENV	23%	65%	91%	53%
ENPD-TEC	22%	55%	65%	59%
ENPI-EW	39%	26%	63%	98%
ED-EW	29%	0%	0%	53%
DIS-EW	0%	0%	0%	0%
S-ENPD-EW	43%	61%	82%	48%

Figure 3.5: *The resource recovery percentages per scenario.*

By changing the weights from equal weighting (ENPD-EW) to 100% economic (ENPD-ECN), a decrease in EAC (-1.6 M€/year) and increase in PIG (+6 M€ /year), due to higher water recovery percentages (+13%), was observed resulting in a lower economic impact. However, the generated treatment train had a higher impact on all the environmental indicators (+0.6 dB, +4 odour, +1.4 ha) and the worst technical score (5.6 flexibility). When the social dimension was exclusively prioritised (ENPD-SOC), the generated treatment train did not show notable improvement either in the scores of the social indicators compared to those of ENPD-EW or in the recovery percentages. Nevertheless ENPD-SOC had a lower EAC (−1.4 M€/year) but also PIG (−1.5 M€/year) and a slightly higher overall environmental impact. Changing the weighting to 100% environmental (ENPD-ENV), resulted in the treatment train with the lowest land requirement (7.6 ha) of all large-scale scenarios that recover resources but one of the lowest COD recovery percentages (23%). The economic impact of ENPD-ENV increased substantially, mainly due to the EAC being five times greater than the EAC of ENPD-EW while the PIG remained in the same range. Setting the weights to 100% technical (ENPD-TEC) gave the best technical score of all scenarios but at the expense of all other sustainability dimensions including the recovery percentages of COD, TN and TP (-16%, -11%, -27%, respectively). Accordingly, considering only one dimension can seriously reduce results for the other dimensions and even reduce the resource recovery potential. The tool supports the evaluation of the impact of decision-maker's priorities via criteria weighting on feasibility and efficiency of resource recovery, which has been reported as necessary but not realised [48].

Targeting different resources to recover, or not prioritising the recovery of any resources, affected sustainability impact and also the amount of resources recovered. Choosing to recover irrigation water (ENPI-EW) instead of drinking water (ENPD-EW) led to the highest amount of recovered water (98%) and the only case with a positive economic impact (a higher PIG, 27 M€/year than EAC, 9.6 M€/year). From an environmental and social point of view, ENPI-EW scored better than ENPD-EW. When only drinking water and energy were targeted (ED-EW) the EAC (-11 M€/year) as well as PIG (-2 M€/year) was lower than when nutrients were also recovered (ENPD-EW). The PIG was lower as nutrients were not recovered, and the mass of recovered COD was lower. From a social perspective, acceptability was lower due to the reduced variety of the targeted resources. When no resources were targeted at all and the water needed to meet discharge regulation (DIS-EW) the economic impact was low, but still negative (higher EAC than PIG). The potential noise emissions (19.9 dB) and land requirement (1 ha) of DIS-EW were the lowest of all the other large-scale scenarios. Conversely, because no resources are being recovered, the acceptability (0.1) of this scenario was the lowest of all scenarios. This can be explained by the fact that [149] formulated acceptability as an indicator such that recovery is preferred over discharge, despite the risks associated with the recovery and reuse of recovered resources. In the literature, most studies provide technical and at most economic and/or environmental impact analysis for predefined, real or hypothetical train configurations [185, 50, 137] while supporting decision-makers to find the most advantageous scenario in terms of four-dimensional sustainability and recovered resources is much needed [48, 186].

For the small-scale resource recovery scenario (S-ENDP-EW), the percentage of recovered nutrients and water is slightly lower ($-5\%, -10\%, -5\%$ for TN, TP and water, respectively) than large scale resource recovery scenario (ENPD-EW). This small scale scenario also has a distinctly lower economic impact (-48.6 M€/year EAC, -26.2 M€/year) than that of ENDP-EW, yet counter intuitively the affordability was also lower. This contradiction can be explained by the fact that affordability takes into account scale differences while EAC and PIG do not. Thus, EAC and PIG are not directly comparable for the large and small scale scenarios unless these are evaluated per population equivalent (PE) or m^3 of influent treated. This proves that the model presented in this study responds to differences in scale and thus the model can also support economies of scale evaluations, a much needed ability for decision-making about for example the degree of decentralisation [187]. Similarly, land footprint of S-ENDP-EW is significantly lower than the one of ENDP-EW which for a fair comparison should also be evaluated per PE or m^3. The impact of all other indicators are not a function of scale and can directly be compared.

A large number of unit processes and combinations thereof are viable options for not only wastewater treatment but also the recovery of many different resources. The current pace of research and development of emerging technologies as well as recoverable resources [48] will result in an exponential increase in the solution alternatives. Thus the case-specific optimum solution for resource recovery from wastewater will therefore become less obvious. However, as also demonstrated in this study, decision support tools with comprehensive evaluation methods can be of great help in efficiently and effectively exploring the vast range of alternative solutions [188], where all unit processes get equal chance to be selected and proposed for implementation. Nevertheless, the optimum solution for a given scenario is very much dependent on (i) the consistency of the information per unit process in the knowledge library and (ii) the evaluation criteria chosen by the user. A unit process can be considered in the decision-making process only if all the required information for impact assessment is available [189], which can be difficult to collect if the process is new or these details are not available due to commercial sensitivity [149]. Finally, only an assessment that simultaneously considers four dimensional sustainability, which covers people, planet, and profit related aspects, will ensure that rational and sustainable decisions are made for resource recovery from urban wastewater.

3.5 Conclusions and recommendations

This study presents the conceptual framework of the NEREUS DST in a reproducible manner. The DST aims to assist decision-makers (policy makers, technology decision-makers, water authorities) to select the optimal combination of unit processes to recover resources from wastewater considering multi-dimensional sustainability. In this study a weighted Multi-Objective Mixed-Integer Nonlinear Programming (WMOMINLP) model was proposed and implemented to select unit processes forming a treatment train that can recover the targeted water, energy and/or nutrients. The model selects unit processes to accommodate the economic, environmental, social and technical impacts. All of these factors are optimised while accounting the weights assigned by the decision-maker. When it is not possible for the model to find a solution, it returns infeasibility. This implies that the targeted resources cannot be recovered from the given influent quality and quantity with the available unit processes in the knowledge library. While previous studies developed decision-making models for water treatment [78] and at most water recovery [153, 172], this is the first study that presents a transparent and reproducible modelling approach for generating a treatment train to simultaneously recover multiple resources, while considering technological and non-technological aspects. Such approaches are much needed in the field in order to speed up the implementation of resource recovery from urban wastewater [48, 186, 190, 159].

The current model ensures that selected unit processes are compatible with each other by grouping unit processes based on the minimum required and maximum allowed COD levels. This assumption enables finding a solution in a very short computational time (3 seconds) but might limit the solution space. Therefore, future work will focus on extending the framework such that it will incorporate the specific limitations of each individual unit process, i.e. minimum required concentrations of N and P for recovery, to expand the application of the framework. This way it will be possible to generate treatment trains for the recovery of resources from various other types of influent streams such as black- and grey water. Moreover, there is a growing research and interest in recovering other resources such as cellulose, bio-polymers, volatile fatty acids which can also be considered as available resources in the tool [190]. However, such extensions will increase the complexity of the problem and thus using an optimisation solver could have a long computational time. Therefore, a heuristic and meta-heuristic algorithm, commonly used to solve the combinatorial optimisation problems, will be needed to deal with the increasingly complex problem of multi-resource recovery from urban wastewater.

4. EXISTING VERSUS NEW PLANT CONFIGURATIONS

Abstract

Technological developments enable the implementation of recovery of water, energy and nutrients at existing wastewater treatment plants but also with new resource recovery plants. However, the trade-offs between the pro's and con's of recovering resources through existing or new plant configurations, have not been studied in detail. Therefore, in this study, three existing and three new alternative treatment and resource recovery scenarios were compared through a multi-criteria decision analysis approach using key performance indicators (KPIs), belonging to economic, technical, environmental and social criteria. A sensitivity analysis of the influent quality and quantity, plant size, and criteria weighting was carried out to evaluate the effect of these on the scores and ranking of scenarios. The scenario analysis showed that each configuration had its own advantages and disadvantages both at KPI level as well as at criteria level. In the sensitivity analysis, yearly fluctuations in influent quality and quantity did not have any effect on the ranking of scenarios within both criteria and overall ranking, but changing plant size and criteria weights did. At large plant size, the existing configurations scored better than the new ones, while at medium and small plant size the new configurations scored better. An increase in the weight assigned to the economic criterion results in higher ranks for the existing configurations, while an increase in weight assigned to the environmental criterion results in higher ranks for the new configurations. The results of this study can be used in decision-making frameworks and tools for systematic/holistic evaluation and design of plant configurations for resource recovery from urban wastewater.

This chapter is under preparation for publication as:
Maria O. van Schaik, Seda Sucu, Djamila Ouelhadj, Wei-Shan Chen, Hans J. Cappon and Huub H.M. Rijnaarts. A comparison between new and existing plant configurations for resource recovery from urban wastewater - The trade-offs between sustainability criteria and their sensitivity.

4.1 Introduction

Wastewater contains valuable organic and inorganic components that can be either directly or indirectly recovered for reuse [52] thus supporting circularity of resources. The most commonly recovered resources from urban wastewater include energy, nutrients, and different qualities of water [34, 74, 13, 191]. Water can be recovered for different purposes including irrigation, industry and even drinking [192, 35, 28]. Already for decades energy has been recovered from urban wastewater in the form of biogas, which is often immediately converted into electricity and heat [13, 38, 39]. Nutrients, mostly phosphorous but lately also nitrogen, are most commonly recovered from digested biodegradables [193]. Other recoverable resources are i.a. hydrogen, polymers, cellulose, volatile fatty acids, and pigments or biofuels via microalgae [194, 195, 196, 197, 198, 37].

Drivers and barriers to implement resource recovery can differ depending on geographical location and cultural context. In developed countries the main drivers of resource recovery are ageing infrastructure and increasingly stringent regulation, which implies upgrading or replacing existing infrastructure [89, 199, 33, 7]. In Western Europe, climate change and concepts like sustainability and circular economy have been pushing resource recovery high on the agenda of decision-makers [200, 143, 201, 202, 203, 204]. In developing countries, the lack of sanitation [205] or inadequate treatment technology [34] requires implementation and improvement of wastewater treatment facilities. Universally used indicators in the context of resource recovery from urban wastewater are recovery efficiencies, resource demand-supply ratios, and acceptability of the recovered resources [206, 202, 207, 204].

The number and amount of resources that can be recovered from a single treatment plant are often limited [208]. Therefore, to ensure successful implementation of resource recovery from urban wastewater, more integrated and context-specific impact evaluations are needed [186]. For this, simultaneous evaluation of technical, economic, environmental and social impacts is recommended [190, 202, 100, 149]. Studies that simultaneously explore all impacts often focus on the recovery of a single resource [71, 72], some with a system boundary exceeding the treatment train [209]. Additionally, some of these studies often use qualitative methods to evaluate processes and treatment trains [73] or just present their advantages and disadvantages without using clearly defined criteria and indicators [74]. Studies employing quantitative methods most commonly evaluate the environmental impact or sustainability of resource recovery from urban wastewater via life-cycle assessment (LCA) or related approaches [54, 210, 3, 211, 212, 213, 214]. However, many studies focus only on the recovery and reuse of one particular resource [54, 212, 214] while a limited number of these studies benchmark the results against conventional wastewater treatment plants (WWTP) [54, 211]. Finally, several authors have demonstrated that scale (plant size) has an effect on technical, economic, environmental and social impacts of wastewater treatment facilities [109], yet few studies evaluate the impact of scale (plant size) on multi-resource recovery [210, 215]. Thus, literature comparing the recovery of multiple resources from urban wastewater with conventional wastewater treatment is fragmented in terms of the recovered resources, the approaches used, and the considered criteria.

Therefore, the aim of this study is to understand the trade-offs between new and exiting configurations for resource recovery, representing different scenarios, in terms of four-dimensional sustainability covering technical, economic, environmental, and social criteria. The configurations were compared at the level of key performance indicators (KPIs), criteria and overall score (ranking). The nature of the KPIs allowed for observing the impact of changes in the recovered resources, influent quality and quantity, and the treatment plant size. A multi-criteria method was subsequently applied to consider decision-makers' preferences through weighting both the KPIs and the criteria.

4.2 Materials and methods

To understand the trade-offs between new and existing configurations for resource recovery, six scenarios were compared by using a multi-criteria decision analysis (MCDA) approach considering a set of technical, economic, environmental and social key performance indicators (KPIs). The KPIs were quantified according to the definitions and mathematical formulations proposed in Chapter 2. In the MCDA approach, a normalisation method was employed to evaluate these KPIs simultaneously. The KPIs are presented in Section 4.2.1 and the applied normalisation method is presented in Section 4.2.2. The comparison of treatment plants consists of two parts:

- A scenario analysis with three different resource recovery plants and three different wastewater treatment plants with and without resource recovery. The WWTP scenario without resource recovery is used as a reference (benchmark).

- A sensitivity analysis of these six treatment plants to (i) variations in wastewater flow and concentration, (ii) treatment plant size (small, medium and large), and (iii) KPI and criteria weights.

These parts are explained in the following sections.

4.2.1 Key performance indicators

This study employed a set of eleven key performance indicators (KPIs) that enabled a quantitative plant-wide analysis and comparison of scenarios. Table 4.1 presents the complete list of used KPIs accounted for in this study per criterion. The parameters and the sources of the data required to quantify the KPIs are provided in Appendix B.1.

Table 4.1: *The KPIs from Chapter 2 used for scenario comparison.*

Criteria	Indicator	Acronym	Unit
Technical	Reliability	REL	-
	Flexibility	FLEX	-
Economic	Capital expenditure	CAPEX	euros
	Operational expenditure	OPEX	euros/year
	Willingness to pay	WTP	-
	Potential income generation	PIG	euros
Environmental	Odour emission potential	OEP	-
	Noise emission potential	NEP	dB
	Footprint	FPT	m^2
Social	Acceptability	ACC	-
	Affordability	AFF	-

4.2.2 Normalisation method of KPIs for comparison

In this study the normalisation method applied by [100] was used to create composite indicators which could then be used in criteria-based and overall evaluations. The method implied differentiating between positive (the higher the better) and negative (the lower the better) KPIs (Equation 4.1 and 4.2, respectively). This method enabled the normalisation of the KPI values (IN, unitless value between 0 and 1, the higher the better) and to aggregate these values of the relevant KPIs per criterion such that scores representing the impacts per criterion could be calculated. This step was necessary to compare scenarios at criterion level and eventually at overall score level.

$$IN_{ip} = \frac{I_{ip} - I_p^{min}}{I_p^{max} - I_p^{min}} \tag{4.1}$$

$$IN_{in} = \frac{I_n^{max} - I_{in}}{I_n^{max} - I_n^{min}} \tag{4.2}$$

where I_{ip} and I_{in} are the actual values of the positive KPI p and negative KPI n for scenario i, I_p^{min} and I_n^{min} are the minimum value per positive and negative KPI (amongst scenarios), I_p^{max} and I_n^{max} are the maximum values per negative KPI (amongst scenarios).

For scenario analysis, flow and concentration sensitivity analysis, and weight impact analysis the minimum and maximum values of the six scenarios were used to obtain the scores (the IN values). For plant size impact analysis the minimum and maximum values of all 18 scenarios (six scenarios and three sizes) were used to obtain the scores which enabled the comparison per scenario (between sizes) and per size (between scenarios).

4.2.3 Scenario analysis

Resource recovery and wastewater treatment plants

Two real-life plant configurations were used to compare resource recovery from wastewater and conventional wastewater treatment. The resource recovery plant (RRP) represents one of the NEREUS project demonstration plants located in The Netherlands which simultaneously recovers several resources: (i) water for irrigation, (ii) energy in the form of biogas, represented by organic matter (COD), (iii) nitrogen in the form of algae biomass represented by total nitrogen (TN), and (iv) phosphorus, represented by total phosphorus (TP). Since at this NEREUS RRP the phosphorous recovery option was still under research, in this study the recovery of phosphorus in the form of struvite was chosen. The conventional wastewater treatment plant (WWTP), used as a benchmark for comparison, represents the configuration of an existing large WWTP from The Netherlands.
Table 4.2 presents the unit processes (UPs) per plant and the sources of the data used per UP. The process flow diagrams of both plants are presented in Figure 4.1 and the data per process are given in Appendix B.2.

The data per UP were mostly obtained from the database of [75]. Missing data per UP as well as data required per KPI were searched for in literature or provided by the NEREUS Interreg 2 Seas project partners. Context (type of location and country) and resource (quality) related data, mostly representing regulation, legislation or directives, were acquired from literature.

Table 4.2: The unit processes (UPs) per plant and the sources of the data.

Processes	UPs considered in this study	Acronyms	Main data source
WWTP - WWTP Walcheren			
Pre-treatment	Bar screen	BS	[75]
Pre-settling	Sedimentation with coagulant	SwC	[75]
Activated sludge with enhanced P removal	Low loaded activated sludge with denitrification and secondary sedimentation	ASwD	[75]
	Enhanced biological phosphorus removal	EBPR	[75]
RRP - NEREUS pilot plant Evides Industriewater			
Drum sieves		DS	[75] data for bar screen
Electrocoagulation		EC	[75] data for Flocculation
Nanofiltration		NF	[75]
Reverse osmosis		RO	[75]
Anaerobic digestion		AD	[75]
Struvite precipitation		SP	[75] data for P-precipitation
Algae culture		AC	[75] data for nanofiltration

Six (two default and four hypothetical) scenarios based on these two plants were used to evaluate the advantages and disadvantages of recovering certain resources. The default WWTP scenario was used as a benchmark. The specifications of each scenario and the resources recovered per scenario are presented in Table 4.3.

The influent

The influent used for simulating the impacts of the scenarios was the influent from WWTP Walcheren, The Netherlands, a conventional urban wastewater stream. The data which were not available from WWTP Walcheren were taken from literature. Table 4.4 presents the influent characteristics, the data used in the analysis, and the data sources. The scenario analysis was carried out using yearly average concetrations ($C_{yearlyaverage}$), while the confidence interval (CI), calculated using Equation 4.3 and representing yearly fluctuations, was used for sensitivity analysis.

$$CI = C_{yearlyaverage} \pm 1.96 * \frac{SD}{\sqrt{N_{DP}}} \tag{4.3}$$

where ± 1.96 represents the 2.5 and 97.5 %ile values, SD is the standard deviation, N_{DP} is the number of data points.

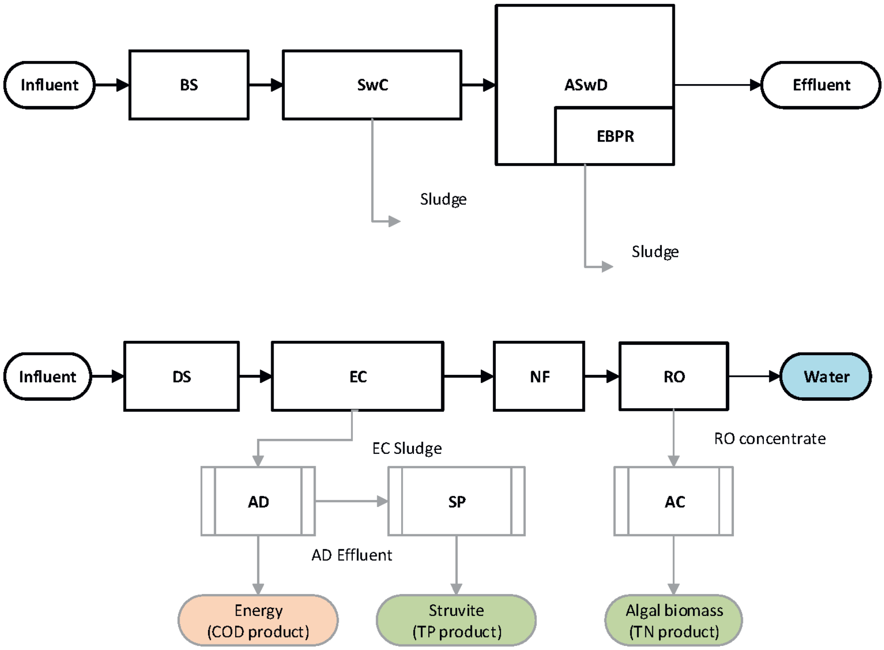

Figure 4.1: *Schematic process flow diagrams of the two plants. Top: WWTP default configuration, bottom: RRP default configuration. Acronyms are provided in Table 4.2.*

Table 4.3: *Scenarios for resource recovery from urban wastewater.*

Scenario		Specification	Water	Nitrogen	Energy	Phosphorous
1	RRP	Resource recovery plant - default configuration	x	x	x	x
2	RRPw/oP	Resource recovery plant without phosphorous recovery	x	x	x	-
3	RRPw/oPE	Resource recovery plant without phosphorous and energy recovery	x	x	-	-
4	WWTP (bench-mark)	Wastewater treatment plant - default configuration	-	-	-	-
5	WWTPwE	Wastewater treatment plant with en-ergy recovery (with AD)	-	-	x	-
6	WWTPwEP	Wastewater treatment plant with energy and phosphorous recovery (with AD and SP)	-	-	x	x

Table 4.4: Influent quality data accounted for in the scenario and sensitivity analysis.

Influent characteristic	Acronym	Unit	Annual average	CI-yearly fluctuations	Data source
Flow rate	Q	m^3/h	1506	1262 - 1750	WWTP Walcheren
Population equivalent	PE	-	144241*	120872-167611*	Calculated
Organic matter	COD	mg/L	517.2	474.4 - 560	WWTP Walcheren
Total nitrogen	TN	mg/L	55.7	50.6 – 60.7	WWTP Walcheren
Total phosphorous	TP	mg/L	7.03	6.4 – 7.6	WWTP Walcheren
Total suspended solids	TSS	mg/L	258.6 **	-	Wastewater characteristics in Europe - A survey
Heavy metals (Cu, Pb, Zn)	HM	mg/L	0.48 ***	-	Wastewater characteristics in Europe - A survey
Pathogens	*E. coli*	cfu/100mL	1.4 x 107	-	RIVM, 2017

*(Q m^3/h x COD mg/L x 24 h/d) / (54 g BOD/person/d x 2.4 g COD/g BOD)
**COD (mg/L) from WWTP Walcheren x 0.5
***Sum of concentrations of Cu, Pb and Zn

4.2.4 Sensitivity analysis

Flow and concentration

A sensitivity analysis was carried out to evaluate the effect of changing flow (influent quantity) and concentration (influent quality), representing yearly fluctuations, on the scores per key performance indicator (KPI), per criterion and on the overall scores. To analyse the sensitivity of KPIs to flow, in cases Q(-) and Q(+) the flow was varied at two levels, while the concentration of pollutants was kept constant. Similarly, for the sensitivity analysis to concentrations, in cases Cs(-) and Cs(+) the concentrations were varied at two levels, Cs(-) and Cs(+), while the flow was kept constant. These variations were performed for each of the six scenarios as described in Table 4.5. The score per KPI was obtained by normalising over all six scenarios per case, using the minimum and maximum values per specific case. The score per criterion was then obtained using equal weights for the relevant KPIs. The overall score represents the sum of scores for all four criteria with equal weights for each criterion. The relative standard deviation (RSD) was used to evaluate the impact of increasing flow or concentrations on the values of the KPIs (not the sores) and was calculated shown in Equation 4.4, 4.5, and 4.6. The RSD was calculated per KPI for each scenario separately for the flow variation and concentration variation cases, both with respect to the base case (BC).

Table 4.5: *The cases for sensitivity analysis.*

Sensitivity cases	Description
Base case (BC)	Annual average flow and concentrations
Q(-)	2.5%ile flow and annual average concentrations
Q(+)	97.5%ile flow and annual average concentrations
Cs (-)	Annual average flow and 2.5%ile TSS, COD, TN and TP concentrations; annual average HM and E. coli concentrations.
Cs (+)	Annual average flow 97.5%ile TSS, COD, TN and TP concentrations; annual average HM and E. coli concentrations.

$$RSD_{KPI_{i,c}} = \frac{SD_{KPI_{i,c}}}{AVG_{KPI_{i,c}}} * 100\% \tag{4.4}$$

$$SD_{KPI_{i,c}} = \sqrt{\frac{\sum_c (KPI_{i,c} - AVG_{KPI_{i,c}})^2}{n_c}} \tag{4.5}$$

$$AVG_{KPI_{i,c}} = \frac{\sum_c KPI_{i,c}}{n_c} \tag{4.6}$$

where i is scenario, c is the case, and n_c is the number of cases.

Plant size

For several decades treatment plant size has been an important topic for wastewater treatment and resource recovery, especially in the context of economies of scale [109]. Therefore, this study evaluated the impact of plant size on the KPIs, criteria and overall score. For this, an average medium and small size plant (determined by flow and PE, Table 4.6) from The Netherlands [216] were chosen to be compared with the BC scenarios which represent an average large size plant in The Netherlands. The population equivalent (PE) per plant was estimated based on the the chemical oxygen demand load (COD in g/day), biological oxygen demand (BOD) per person per day (54 g/person.day of BOD) and the ratio be-tween chemical and biological oxygen demand from WWTP Walcheren (average COD:BOD of 2.40). The influent quality (concentrations) in these cases was the same as in the BC scenarios. To analyse the impact of the plant size, the KPI values were first divided by the flow. Then the minimum and maximum of these KPI values of all 18 scenarios (six scenarios and three sizes) were used to obtain the scores. This method enabled the comparison per scenario (between sizes) and per size (between scenarios).

Table 4.6: The plant size specifications.

	Unit	Large (L)	Medium (M)	Small (S)
Flow (Q)	m^3/h	1506	300	30
Population equivalent (PE)*	PE	144241	28733	2873

*(Q m^3/h x COD mg/L x24 h/d) / (54 g BOD/person/d x 2.4 g COD/g BOD)

Weights

The scenario analysis as well as the sensitivity analyses of flow, concentration, and plant size were carried out by equal weighting of criteria and KPIs. Two different weighting approaches were used to gain insight about the sensitivity of the results to different weights. Firstly, NEREUS Interreg 2 Seas project partners provided weights per criterion and per KPI via email exchange (Table 4.7). Secondly, a systematic weighting approach with single and multiple criteria combined (Table 4.8) was performed. For weight impact analysis the normalisation of the KPI values was done with the minimum and maximum values of the six scenarios.

Table 4.7: Weights provided by the decision-makers (NEREUS Interreg 2 Seas project partners).

Criteria	KPIs	Weights									
		Partner 1		Partner 2		Partner 3		Partner 4		Partner 5	
		Criteria	KPIs	Criteria	KPIs	Criteria	KPIs	Criteria	KPIs	Criteria	KPIs
Econ	CAPEX	40%	40%	25%	40%	25%	25%	30%	50%	30%	25%
	OPEX		40%		40%		25%		30%		30%
	PIG		0%		20%		25%		15%		20%
	WTP		20%		0%		25%		5%		25%
Tech	REL	40%	80%	35%	60%	25%	80%	40%	75%	30%	50%
	FLEX		20%		40%		20%		25%		50%
Env	OEP	15%	50%	25%	40%	25%	33%	20%	40%	30%	35%
	NEP		50%		30%		33%		40%		35%
	FPT		0%		30%		33%		20%		30%
Soc	ACC	5%	50%	15%	50%	25%	50%	10%	30%	10%	50%
	AFF		50%		50%		50%		70%		50%

Table 4.8: *Systematic weights per criterion.*

	Two-criteria weight evaluation																	
Econ	75%	75%	75%	50%	50%	50%	25%	25%	25%									
Tech	25%			50%			75%			75%	75%	50%	50%	25%	25%			
Env		25%			50%			75%		25%		50%		75%		75%	50%	25%
Soc			25%			50%			75%		25%		50%		75%	25%	50%	75%

	Three-criteria weight evaluation													Equal weight	Single weight			
Econ	50%	50%	50%	25%	25%		25%	25%			25%	25%		25%	100%			
Tech	25%		25%	50%	50%	50%	25%		25%	25%		25%		25%		100%		
Env	25%	25%		25%		25%	50%	50%	50%	25%	25%			25%			100%	
Soc		25%	25%		25%	25%		25%	25%	50%	50%	50%		25%				100%

4.3 Results

In this section the results for the six scenario evaluations and sensitivity analyses are presented in detail. The results of the six scenarios include the results per KPI, per criterion and the overall scores.

4.3.1 Scenario analysis

Of all six scenarios considered, the benchmark WWTP had the highest overall score (Table 4.9). Per criterion, the WWTP scored only third best for the economic criterion, second best for technical and environmental criteria and best for the social criterion. The RRP, simultaneously recovering water, energy, and nutrients (TN and TP), had the lowest overall score. This scenario scored relatively low especially for economic and technical, yet scored equally high as the WWTP for the social criterion.

To enable a more detailed comparison between all six scenarios, the values per KPI were benchmarked against the WWTP scenario (Figure 4.2). The results per KPI are presented and discussed in detail per criterion in the following subsections.

Technical criterion

The technical impact was evaluated through two KPIs: reliability (REL) and flexibility (FLEX). The REL, expressed in percentage, refers to the percentage of the time that the plant delivers the required performance. Evaluations for the six scenarios showed that the WWTP scenarios are on average 25-30% more reliable than the RRP scenarios. One of the reasons for this is the fact that the RRP scenarios have a higher number of unit processes, some of which (i.e. EC and algae)

Table 4.9: *The criteria and overall scores* for the six scenarios presented in Table 4.3. The colour coding* is done horizontally, so per criterion, thus comparing different plant types.*

Scores	RRP	RRPw/oP	RRPw/oPE	WWTP	WWTPwE	WWTPwEP
Econ	0,474	0,483	0,422	0,547	0,675	0,614
Tech	0,212	0,555	0,550	0,675	0,726	0,349
Env	0,526	0,559	0,681	0,625	0,370	0,316
Soc	0,500	0,496	0,495	0,500	0,496	0,465
Overall score	0,428	0,523	0,537	0,587	0,567	0,436

*Interpretation for the scores: the higher the score the better; colour code: red=low score, green=high score.

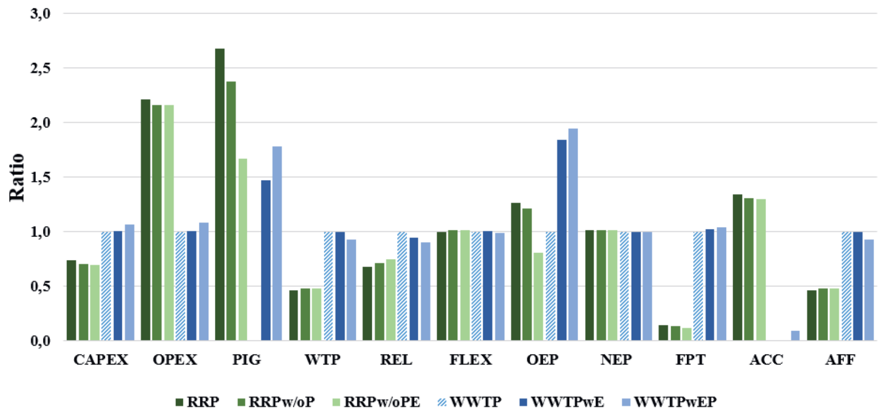

Figure 4.2: *The results per KPI for the six scenarios benchmarked against WWTP.*

have a lower technology readiness level (TRL) for urban wastewater treatment applications. In terms of flexibility, all six scenarios showed similar flexibility, meaning that all scenarios can handle comparable influent concentration changes. Overall, for the technical criteria WWTPwE scored the highest, while RRP the lowest of all scenarios (Table 4.9, results per criteria).

Economic criterion

The economic KPIs used in this study were: capital expenditure (CAPEX), operational expenditure (OPEX), potential income generation (PIG) and willingness to pay (WTP). The three RRP scenarios showed approximately 30% lower CAPEX than the WWTP, mainly due to the higher CAPEX of the activated sludge unit (ASwD) in the WWTP. Yet the OPEX of all RRP scenarios were over two times larger than the OPEX of WWTP, as RRP scenarios make use of energy intensive processes including NF and RO for recovering water. Since the WWTP does not recover any resources, the scenario had a PIG of 0 €/yr. However, to enable benchmarking against WWTP, the value of 0.1 €/yr was used to avoid a division by zero (0 €/yr PIG). This way, of all six scenarios considered in this study, RRP had the highest PIG. In terms of WTP, the WWTP scenarios showed about two times higher WTP in comparison with the RRP scenarios as WTP is negatively impacted by the OPEX. Accordingly, the WWTP scenarios scored economically better than the RRP scenarios, with WWTPwE obtaining the highest score for the economic criterion of all six scenarios (Table 9, overall scores).

Environmental criterion

The environmental impact in this study was evaluated through odour emission potential (OEP), noise emission potential (NEP), and land footprint (FPT). The RRPw/oPE and WWTP had the lowest OEP of all scenarios as they were the only scenarios without energy recovery which generally implies processing streams high in COD concentrations. In terms of NEP, all scenarios showed similar values, with the RRP scenarios showing slightly higher NEP than the WWTP scenarios. The FPTs of the RRP scenarios were almost ten times lower than the FPTs of the WWTP scenarios, despite the greater number of processes. This is mostly because the processes involved in the RRP have a lower FPT per m^3 of influent. The scenario with the highest overall environmental score was RRPw/oPE, followed by the benchmark WWTP.

Social criterion

The social KPIs in this study were acceptability (ACC), and affordability (AFF). In terms of ACC, the RRP scenarios showed 1000 times higher ACC values in comparison with WWTP, mostly due to increased capacity of the RRP scenarios to remove HM from the recovered water. Of the WWTP scenarios, WWTPwEP showed the highest ACC. This is related to the fact that this KPI favours resource recovery (Chapter 3 or [217]). The three WWTP scenarios had an approximately two times higher AFF in comparison with the RRP scenarios. Overall, RRP and WWTP had the same social score while WWTPwEP scored lowest of all scenarios.

4.3.2 Sensitivity analyses

Flow and concentration

With yearly fluctuations in influent flow and concentrations the KPI values changed (Table 4.10) but these changes did not affect the ranking of scenarios within both criteria and the overall ranking. Some of the indicators considered in this study were only affected by changes in flow (e.g. CAPEX, OPEX, FPT), some were affected by changes in both flow and concentration (e.g. PIG, WTP, OEP, ACC, AFF), while others were not affected by changes in either flow or concentration (ie REL, FLEX, NEP). This is substantially dependent on the KPIs' mathematical formulation as well as on the UP database. From the UP database used in this study, CAPEX, OPEX and FPT of UPs are functions of flow [75]. A flow variation of 16.2% impacted the OPEX of the RRP scenarios the most (RSD of 17.52-17.66%). For water recovery, the RRP scenarios are making use of processes such as NF and RO with energy consumption highly dependent on flow [75]. Concentration variations of 8-9% impacted PIG of WWTPwEP the most (RSD of 8.32%), as the removed COD and TP by the second and the third UP in the WWTP scenario (SwC and ASwC in Figure 4.1), ending up in the primary and secondary sludge, while in the RRP scenario only the removed COD and TP by the second UP (EC in Figure 4.1) were considered for recovery. Despite the variations (RSDs) of the values per KPI, the considered variations in flow and concentration did not affect the criteria and overall scores per scenario (RSD 0-1%).

Table 4.10: *The relative standard deviations (RSD, %) of the KPI values over the cases considered in the sensitivity analysis (Q(-), Q(+), Cs(-), Cs(+)) for the six scenarios*. RRP, RRPw/oP, RRPw/oPE, WWTP, WWTPwE, and WWTPwEP.*

	RRP		RRPw/oP		RRPw/oPE		WWTP		WWTPwE		WWTPwEP	
	BC, Q(-), Q(+)	BC, Cs(-), Cs(+)	BC, Q(-), Q(+)	BC, Cs(-), Cs(+)	BC, Q(-), Q(+)	BC, Cs(-), Cs(+)	BC, Q(-), Q(+)	BC, Cs(-), Cs(+)	BC, Q(-), Q(+)	BC, Cs(-), Cs(+)	BC, Q(-), Q(+)	BC, Cs(-), Cs(+)
CAPEX	13,13%	0,00%	12,99%	0,00%	13,03%	0,00%	10,69%	0,00%	10,67%	0,00%	10,99%	0,00%
OPEX	17,52%	0,00%	17,65%	0,00%	17,66%	0,00%	12,72%	0,00%	12,71%	0,00%	12,77%	0,00%
PIG	16,20%	5,04%	16,20%	4,60%	16,20%	3,05%	-	-	16,20%	8,28%	16,20%	8,32%
WTP	0,16%	8,27%	0,11%	8,27%	0,10%	8,27%	4,31%	8,28%	4,32%	8,28%	4,17%	8,28%
REL	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
FLEX	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
OEP	16,20%	8,28%	16,20%	8,28%	16,20%	8,28%	16,20%	8,28%	16,20%	8,28%	16,20%	8,28%
NEP	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
FPT	6,48%	0,00%	5,82%	0,00%	4,82%	0,00%	16,26%	0,00%	16,24%	0,00%	16,24%	0,00%
ACC	0,00%	0,49%	0,00%	0,28%	0,00%	0,28%	3,74%	3,74%	0,66%	0,66%	0,04%	8,00%
AFF	0,16%	8,27%	0,11%	8,27%	0,10%	8,27%	4,31%	8,28%	4,32%	8,28%	4,17%	8,28%

*RRP: recovery of water, nitrogen, energy and phosphorus; RRPw/oP: recovery of water, nitrogen and energy; EEPw/oPE: recovery of water and nitrogen; WWTP: water treatment for discharge and no recovery; WWTPwE: water treatment for discharge and recovery of energy; WWTPwEP: water treatment for discharge and recovery of energy and phosphorus.

Plant size

The criteria and overall scores for the six scenarios at large (L), medium (M), and small (S) scale are presented in Table 4.11. Overall, the large scale seemed most advantageous for all scenarios, for almost all criteria, except for technical, and for the overall score. From an economic perspective, the decrease in size impacts the WWTP scenarios the most (RSD 62-81%) and the small scale WWTP had the lowest economic score. Size had no impact on the technical criterion as none of the technical KPIs is a function of flow. Environmentally, size makes the greatest difference for the RRP scenarios (RSD 32-44%), yet almost no difference for the WWTP scenarios (RSD 0%). The best scoring scenario from an environmental perspective was the WWTP, while the worst scoring was RRP at small size. From a social perspective, size impacted the scores of the WWTP scenarios much more (RSD 95%) than the scores of the RRP scenarios (RSD 15%). The RRP scenarios at large and medium size scored best of all scenarios while WWTP scenarios at medium and small size scored worst of all scenarios. In terms of the overall score, the same trend can be observed: the lower the size the lower the overall scores for all scenarios (RSD 20-35%). At large size the WWTP scored best and at small size the RRPw/oPE scored best.

Table 4.11: *The scores* per criterion, overall scores and the relative standard deviation (RSD, %) per scenario over the plant sizes.*

	RRP	RRPw/oP	RRPw/oPE	WWTP	WWTPwE	WWTPwEP
Economic						
BC-L	0,772	0,752	0,687	0,729	0,864	0,864
M	0,728	0,711	0,647	0,524	0,658	0,666
S	0,417	0,413	0,351	0,046	0,179	0,175
RSD	30%	30%	33%	81%	62%	62%
Technical						
BC-L	0,212	0,555	0,550	0,675	0,726	0,349
M	0,212	0,555	0,550	0,675	0,726	0,349
S	0,212	0,555	0,550	0,675	0,726	0,349
RSD	0%	0%	0%	0%	0%	0%
Environmental						
BC-L	0,530	0,561	0,681	0,784	0,534	0,482
M	0,484	0,514	0,635	0,785	0,534	0,483
S	0,200	0,231	0,352	0,786	0,535	0,484
RSD	44%	41%	32%	0%	0%	0%
Social						
BC-L	0,673	0,666	0,665	0,500	0,498	0,488
M	0,635	0,630	0,629	0,255	0,254	0,265
S	0,500	0,493	0,492	0,012	0,013	0,037
RSD	15%	15%	15%	95%	95%	86%
Overall score						
BC-L	0,547	0,633	0,646	0,672	0,655	0,546
M	0,515	0,603	0,615	0,560	0,543	0,441
S	0,332	0,423	0,436	0,380	0,363	0,261
RSD	25%	21%	20%	27%	28%	35%

*Interpretation for the scores: the higher the score the better; colour coding per criterion: lightest=lowest score, darkest=highest score; colour coding overall score: red=low score, green=high score.

Weights

Accounting for the weights provided by the NEREUS project partners did not considerably impact the ranking of scenarios (Table 4.12). When accounting only for the weights per criterion, for each of the partners RRP showed the worst overall score, while either WWTP or WWTPwE showed the best overall score. This can be explained by the fact that almost all partners gave less importance to the social and environmental criteria, while the RRP scored better for these criteria (see score per criteria in Table 4.9). Accounting for both KPI and criteria weights (Table 4.7) resulted in an even greater difference between the best and worse overall scores as well as some shifts in the ranking. Even though most of these partners wish to recover resources with new configurations, this is not reflected in the results using their preferred weights. For partner 1, 3, and 4 RRPw/oP became slightly less advantageous than WWTPwEP. The reasons for this shift may be explained by the difference in equal weights and the weights provided by the partners. Per partner the differences in weights were:

- Partner 1: PIG (0% instead of 25%), REL (80% instead of 50%), and FPT (0% instead of 33%);
- Partner 3: REL (80% instead of 50%);
- Partner 4: PIG (15% instead of 25%), REL (75% instead of 50%), FPT (20% instead of 33%), and ACC (30% instead of 50%).

The impact of weights on the scenario ranking was further evaluated through a systematic weighting approach as explained in Section 4.2.4. The results are presented in Table 4.13. Depending on the combination of two criteria (two-criteria evaluation) and the assigned weights, a scenario scored better (Table 4.13, green colour) or worse (Table 4.13, red colour). The same could be observed for the different combinations of three criteria (three-criteria evaluation). Nevertheless, none of the combinations of two or three criteria with the variations in weights resulted in major shifts in scenario ranking in comparison to equal weighting: WWTP and WWTPwE remaining the two most advantageous scenarios and RRP and WWTPwEP the two most disadvantageous scenarios. However, an increase in the weight assigned to the economic criterion results in higher ranks for the WWTP scenarios, especially for the WWTPwEP. Similarly, an increase in weight assigned to the environmental criterion results in higher ranks for the RRP scenarios, especially the RRPw/oPE. The impact of weights is in fact most visible when one-criterion evaluation is carried out (100% weight for each criterion).

Table 4.12: *Overall scores* of BC scenarios with (A) equal weights (for KPIs and criteria), (B) weights provided by the partners per criteria (equal weights per KPI within one criterion) and (C) weights provided by the NEREUS project partners for KPIs and criteria. The colour coding** is used for the whole matrix, thus comparing the results per partner as well as plant types.*

	RRP	**RRPw/oP**	**RRPw/oPE**	**WWTP**	**WWTPwE**	**WWTPwEP**
	A – equal weights for indicators and criteria					
BC	0,428	0,523	0,537	0,587	0,567	0,436
	B – partner specific weights only per criterion					
Partner 1	0,378	0,524	0,516	0,607	0,641	0,456
Partner 2	0,399	0,529	0,543	0,604	0,590	0,424
Partner 3	0,428	0,523	0,537	0,587	0,567	0,436
Partner 4	0,382	0,528	0,532	0,609	0,616	0,433
Partner 5	0,414	0,529	0,545	0,604	0,581	0,430
	C – partner specific weights on both criteria and KPIs					
Partner 1	0,247	0,357	0,414	0,780	0,690	0,535
Partner 2	0,407	0,526	0,558	0,614	0,566	0,413
Partner 3	0,395	0,455	0,487	0,634	0,584	0,487
Partner 4	0,339	0,450	0,492	0,686	0,626	0,474
Partner 5	0,392	0,509	0,532	0,628	0,593	0,439

*Interpretation for the scores: the higher the score the better; colour code: red=low score, green=high score.

4.4 Discussion

The applied methodology enabled the comparison of wastewater treatment and resource recovery scenarios at the key performance indicators (KPI), criteria (technical, economic, environmental and social) and higher overall level. The actual advantages and disadvantages of the scenarios were put into perspective by benchmarking the KPI values of alternative scenarios against the existing WWTP. To compare scenarios at criteria and overall level a normalisation method was applied to the KPI values. The effects of influent quality and quantity seasonal variation, plant size, and weights representing decision-makers' priorities on the KPI values were then studied through a sensitivity analysis.

At KPI level, the main drivers and barriers of resource recovery were observed. Based on the evaluation carried out in this study, the drivers of RRP scenarios are potential income generation, footprint and acceptability while the barriers are operational expenditure, reliability and affordability. At the criteria level, the results of this study demonstrated the importance of accounting for environmental and social criteria for the implementation of resource recovery. These two criteria are especially important when medium and small plant sizes are evaluated. Nevertheless, the multi-criteria analysis depends on the KPIs accounted for, their definitions, and the system boundary considered in the evaluation. Especially the economic and environmental criteria could be extended to cover, for example, costs and environmental impact of all side (waste)streams [218, 219]. This way the trade-offs are accounted for at an overall level. Therefore, when analysis is carried out in a transparent manner, with KPIs and their definitions provided, four-dimensional sustainability, covering technical, economic, environmental, and social KPIs, can assure a fair overall evaluation of scenarios.

Influent quality and quantity variations within the limits of seasonal changes had a minor effect on some of the KPI values however without affecting the ranking. This indicates that the applied method is trustworthy when annual flow and concentration averages are used. Treatment plant size had an impact on both criteria and overall scores. All scenarios were less advantageous as the size decreased (lower score), which is in line with for example the economies of scale [220, 109]. A large size WWTP ranked best of all scenarios, while for medium and small sized plants the RRPw/oPE was the most advantageous, meaning that WWTP scenarios are affected more than the RRP scenarios by a change in plant size, especially when the WWTP is retrofitted to recover resources. Such information is especially relevant in the early stages of urban planning and resource multi-sourcing [220, 221]. For a more accurate planning plant size analysis should include the collection and transportation networks as well [222, 223].

Table 4.13: *The overall scores* for the systematic weighting approach and the standard deviation across different plants.*

	RRP	RRPw/oP	RRPw/oPE	WWTP	WWTPwE	WWTPwEP	SD of scores
One-criterion evaluation							
Econ 100%	0,474	0,483	0,422	0,547	0,675	0,614	0,095
Tech 100%	0,212	0,555	0,550	0,675	0,726	0,349	0,196
Env 100%	0,526	0,559	0,681	0,625	0,370	0,316	0,143
Soc 100%	0,500	0,496	0,495	0,500	0,496	0,465	0,014
Two-criteria evaluation							
Econ 100%	0,474	0,483	0,422	0,547	0,675	0,614	0,095
Econ 75% Tech 25%	0,409	0,501	0,454	0,579	0,688	0,548	0,099
Econ 50% Tech 50%	0,343	0,519	0,486	0,611	0,700	0,481	0,122
Econ 25% Tech 75%	0,278	0,537	0,518	0,643	0,713	0,415	0,156
Tech 100%	0,212	0,555	0,550	0,675	0,726	0,349	0,196
Econ 100%	0,474	0,483	0,422	0,547	0,675	0,614	0,095
Econ 75% Env 25%	0,487	0,502	0,487	0,566	0,599	0,539	0,046
Econ 50% Env 50%	0,500	0,521	0,552	0,586	0,523	0,465	0,042
Econ 25% Env 75%	0,513	0,540	0,616	0,605	0,446	0,390	0,089
Env 100%	0,526	0,559	0,681	0,625	0,370	0,316	0,143
Econ 100%	0,474	0,483	0,422	0,547	0,675	0,614	0,095
Econ 75% Soc 25%	0,481	0,486	0,440	0,535	0,630	0,576	0,070
Econ 50% Soc 50%	0,487	0,489	0,459	0,523	0,586	0,539	0,045
Econ 25% Soc 75%	0,494	0,493	0,477	0,512	0,541	0,502	0,022
Soc 100%	0,500	0,496	0,495	0,500	0,496	0,465	0,014
Env 100%	0,526	0,559	0,681	0,625	0,370	0,316	0,143
Env 75% Soc 25%	0,520	0,543	0,635	0,594	0,402	0,353	0,110
Env 50% Soc 50%	0,513	0,527	0,588	0,562	0,433	0,390	0,076
Env 25% Soc 75%	0,507	0,512	0,542	0,531	0,465	0,427	0,043
Soc 100%	0,500	0,496	0,495	0,500	0,496	0,465	0,014
Env 100%	0,526	0,559	0,681	0,625	0,370	0,316	0,143
Tech 25% Env 75%	0,448	0,558	0,648	0,637	0,459	0,324	0,125
Tech 50% Env 50%	0,369	0,557	0,616	0,650	0,548	0,332	0,131
Tech 75% Env 25%	0,291	0,556	0,583	0,662	0,637	0,341	0,157
Tech 100%	0,212	0,555	0,550	0,675	0,726	0,349	0,196
Tech 100%	0,212	0,555	0,550	0,675	0,726	0,349	0,196
Tech 75% Soc 25%	0,284	0,540	0,536	0,631	0,668	0,378	0,148
Tech 50% Soc 50%	0,356	0,526	0,523	0,587	0,611	0,407	0,100
Tech 25% Soc 75%	0,428	0,511	0,509	0,544	0,553	0,436	0,053
Soc 100%	0,500	0,496	0,495	0,500	0,496	0,465	0,014
Three-criteria evaluation							
Econ 50% Tech 25% Env 25%	0,422	0,520	0,519	0,598	0,611	0,473	0,073
Econ 25% Tech 50% Env 25%	0,356	0,538	0,551	0,630	0,624	0,407	0,113
Econ 25% Tech 25% Env 50%	0,435	0,539	0,584	0,618	0,535	0,399	0,085
Econ 50% Tech 25% Soc 25%	0,415	0,504	0,472	0,567	0,643	0,510	0,079
Econ 25% Tech 50% Soc 25%	0,350	0,522	0,504	0,599	0,656	0,444	0,109
Econ 25% Tech 25% Soc 50%	0,422	0,508	0,491	0,555	0,598	0,473	0,062
Econ 50% Env 25% Soc 25%	0,494	0,505	0,505	0,555	0,554	0,502	0,028
Econ 25% Env 50% Soc 25%	0,507	0,524	0,570	0,574	0,478	0,427	0,056
Econ 25% Env 25% Soc 50%	0,500	0,508	0,523	0,543	0,509	0,465	0,026
Tech 50% Env 25% Soc 25%	0,350	0,522	0,504	0,599	0,656	0,444	0,109
Tech 25% Env 50% Soc 25%	0,441	0,542	0,602	0,606	0,490	0,361	0,096
Tech 25% Env 25% Soc 50%	0,435	0,526	0,555	0,575	0,522	0,399	0,070
Four-criteria evaluation (equal weighig)							
Econ 25% Tech 25% Env 25% Soc 25%	0,428	0,523	0,537	0,587	0,567	0,436	0,067

*Interpretation for the scores: the higher the score the better; colour code: red=low score, green=high score.

The evaluations presented are highly dependent on the availability of unit process data, on the country-specific context, and on data related to the recovered resources. Per UP, data (i.e. costs, performance, reliability, etc.) can vary depending on technology supplier, configuration, operation, and influent quality. Additionally, context data can vary per country, even per province or region, and most importantly per type of location, e.g. residential, industrial or natural area. Therefore, the reliance of this method on the data leads to both uncertainties and limitations. Thus accurate decision-making requires extensive data.

4.5 Conclusions and recommendations

This study applied previously defined and mathematically formulated key performance indicators (KPIs) belonging to technical, economic, environmental, and social criteria, to evaluate resource recovery scenarios and benchmark these against existing wastewater treatment. While the multi-criteria evaluation is necessary for a comprehensive impact analysis of scenarios, benchmarking with WWTP provides a meaningful comparison of scenarios and increases understanding of trade-offs made. Form an environmental perspective, the recovery of energy and phosphorous in the RRP scenarios (new configurations) score better than their recovery in the WWTP scenarios (existing configurations). Form a technical or economic perspective the results showed the opposite. From a social perspective, the scores of both RRP and WWTP scenarios were similar.

The recovery of one or more resources in a specific configuration comes with trade-offs. The RRP scenario recovering water, nitrogen and energy showed slight improvement for the economic, technical, and environmental criteria in comparison with the RRP scenario recovering also phosphorus. The recovery of only water and nitrogen in the RRP scenario showed an better (higher) score for the environmental criteria but a worse (lower) score for the economic criteria. The recovery of energy in the WWTP scenario resulted in higher economic and technical but lower environmental and social scores. The recovery of both energy and phosphorus in the WWTP scenario resulted in lower scores for all of the criteria in comparison with WWTP scenarios recovering energy. Therefore the criteria weights impact the evaluation at the overall level. Furthermore, depending on the plant size, recovering resources at new configurations can become more advantageous in terms of four-dimensional sustainability in comparison with existing configurations. Thus multi-criteria evaluation plays an important role in deciding upon the recovery of resources, with a specific configuration at a given plant size.

The reliability of the outcome, however, remains dependent on the reliability of the data used in the evaluation of the configurations. Therefore, future work could evaluate the sensitivity of the results to (i) ranges in process performance [137], (ii) value of recovered product [224], and (iii) future developments in policy and legal frameworks. The latter is especially important as policy and legislation can determine the technical, economic, environmental, and social impact of resource recovery facilities throughout the period that they are designed for [225, 226, 190, 223, 227].

5. Model-based decision-making at process level

Abstract

Existing decision support tools (DSTs) are commonly oversimplifying the process choices by accounting only for average performance, while processes show different performances depending on specifications of the configuration and the chosen operating conditions. This study aims to introduce varying configurations and relevant operating conditions of processes into decision-making without going into complex (mathematical) process performance evaluations. The process used to present this approach is nanofiltration (NF), a promising process for both water and nutrient recovery. An NF model was built and used to generate surface responses of varying capital expenditure (i.e. membrane area, m^2) and operational expenditures (i.e. pumping power, kW) in response to transmembrane pressure (TMP, bar) for two different NF membrane types. The results of this study showed that the selection of NF membranes (i.e. Dow NF90 or Dow NF270) and the operating conditions (i.e. TMP between 4-24 bar) is less dependent on the influent quality than on the targeted resource recovery performance. Yearly fluctuations in influent quality and quantity, resulted in the selection of the same membrane (NF270) and slightly varying TMPs (7-9 bars), indicating that the selected process is robust to seasonal variations. When changing the targets for recovered water quality and quantity, the optimisation model selected different membranes and TMPs, indicating that the selection is sensitive to resource targets. In conclusion, the model in this study is robust where needed and responsive to different resource recovery scenarios when required.

A version of this chapter is under review as:
Maria O. van Schaik, Iarima S. Mendonca, Hans J. Cappon, Wei-Shan Chen, and Huub H.M. Rijnaarts. Integrating process characteristics into model based decision-making for resource recovery - A grey-box approach applied to nanofiltration.

5.1 Introduction

Resource recovery from urban wastewater is not yet widely implemented, despite it being researched and advocated worldwide by many, already for several decades. The reasons behind the lag between research and implementations are manifold. On one hand, conventional wastewater treatment plants (WWTP) were designed to last for decades, even up to a century, and thus there has been little need for substantial updates [228]. On the other hand, the implementation of resource recovery is challenging due to technical, economic, environmental and social aspects related to the processes used and the recovered resources [150, 148]. Moreover, the number of processes capable of recovering different resources from various streams is continuously increasing [51, 43, 7, 28]. All these aspects have increased the complexity of decision-making regarding (i) which resource should be recovered, (ii) where and with which process, and (iii) under what conditions, thus hindering the implementation of resource recovery from wastewater [217].

Decision support tools (DSTs) have been proven to be effective in supporting complex decision-making problems, including problems related to wastewater treatment process selection and treatment train design [199, 229]. Several studies have developed (prototype) mathematical programming models able to select a (specific) number of processes that together form a treatment train recovering the targeted resources from urban wastewater, while accommodating technical, economic, environmental and/or social impact [78, 76, 108, 75, 217]. However, these models incorporate only average or at most minimum and maximum performance settings per process, while most processes can have a range of performances and thus a range of impacts depending on the chosen process configuration and operating conditions [137].

The selection of processes for a treatment train could benefit from a more extended knowledge library per process, including process performance variations with characteristics of configurations and process operations. However, considering multiple performances per process leads to an increase in the number of numerical evaluations [82]. A large number of such numerical evaluations benefit from simple and fast models (or mathematical functions) with an adequate level of detail to cover the desired variations of configurations and operational settings [137]. Therefore, the objective of this study is to demonstrate how the inclusion of more details (in this case, configuration and operational settings) of a single process for resource recovery influences the decision-making at process level. For this, we chose to model nanofiltration (NF), a process interesting for both water and nutrient recovery from urban wastewater [230, 231, 232, 233].

5.2 Theoretical background

NF is a pressure driven process using membranes with properties lying between those of ultrafiltration (UF) membranes and reverse osmosis (RO) membranes [234]. NF is known to reject most organic matter and polyvalent ions, such as phosphate (PO_4^{3-}), while permeating monovalent ions, such as ammonium (NH_4^+), and water [230, 231]. Both ion rejection, represented by solute rejection percentage, and water permeation, represented by water flux, have been found to vary per membrane type and net driving pressure (NDP)[235]. Membrane type is most commonly defined by membrane material and molecular weight cut-off (MWCO, Da).

The ion rejection and permeation in NF membranes is governed by two main mechanisms: steric exclusion-depending on both the solute and pore/opening size, and Donnan exclusion-depending on solute and membrane surface charge [236]. The NF process would be best described by a transition model between solution-diffusion applied to non-porous membranes (i.e. RO) and pore-flow model-applied to porous membranes (i.e. UF) [237]. Even though solution-diffusion models are most commonly used to describe RO processes [238], several studies stated and demonstrated that they can be used to describe NF [239, 235, 240, 241, 242, 243]. [240] evaluated several types of irreversible thermodynamic, solution-diffusion, and pore-flow models for describing organic solvent NF membranes and found solution diffusion-based models to best describe then NF process with irregular voids (i.e. flexible polymer backbone). [242] reviewed models to evaluate membrane integrity and to identify damages in NF and RO membranes and concluded that solution-diffusion is appropriate to use for NF. Therefore in this study the solution-diffusion model was slightly modified and applied to two membranes as described in the following section.

5.3 Methodology

The NF membrane model in this study (Section 5.3.1) represents a grey-box model, combining mechanistic (solution-diffusion) and empirical (estimating water and solute permeability) approaches, which accounts for only relevant variables that are readily available from practice (Jeppsson 1996). The NF model was used to generate surface responses of varying capital expenditures (membrane area, m^2) and operational expenditures (pumping power, kW) in response to transmembrane pressure (TMP, bar). The applicability and relevance of the NF model was then evaluated via an optimisation model (Section 5.3.2) which aims to minimise costs. The optimisation model finds the optimal combination of (i) membrane type and (ii) operating condition to recover the targeted resources by minimising capital and operational expenditures. Two polyamide thin-film membranes, Dow NF90 and Dow NF270, were modelled and used for the optimisation purposes.

5.3.1 Membrane types and model

The specifications of the two membranes modelled in this study, Dow NF90 and Dow NF270, and the data found in literature are presented in Table 5.1. Due to differences in MWCO, these membranes differ mostly in terms of water flux and total nitrogen (TN) rejection, but are equally good in rejecting organic matter (COD) and total phosphorous (TP). In this study, TN and TP represent the most commonly found ions in urban wastewater effluents: ammonium (NH_4^+), nitrate (NO_3^-), and nitrite (NO_2^-) for TN and phosphate (PO_4^{3-}) for TP.

The solution-diffusion model was used for fitting experimental data obtained from literature for the two NF membranes. The parameters fitted were water flux (J_w) and solute rejections (SR) for each of the components of interest: COD, TN, TP. According to the solution diffusion model, flux is a function of water permeability (A) and net driving pressure (NDP) as presented in Equation 5.1 and NDP is a function of transmembrane pressure (TMP) and osmotic pressure difference ($\Delta\pi$) as presented in Equation 5.2.

$$J_W = A * NDP \tag{5.1}$$

$$NDP = (TMP - \Delta\pi) \tag{5.2}$$

However, since all the data used for fitting was obtained with conventionally treated or MBR treated municipal effluent with low conductivity, in this study the osmotic pressure difference ($\Delta\pi$) was neglected. This was also done for practical reasons, as osmotic pressure of the influent and permeate or other related variables such as electrical conductivity are hardly reported in relevant literature. Therefore, in this study Equation 5.1 becomes Equation 5.3.

Table 5.1: *The membranes and the respective data used for modelling and optimisation.*

		Unit	Dow NF90	Dow NF270
Membrane properties				
Material		-	Polymer - Polyamide - Thin-film composite	
MWCO		Da	200	200-400
Influent				
Type		-	Conventionally treated or MBR treated municipal effluent	
Temperature		°C	20-27	14-27
Operation and performance				
TMP		bar	2-20	4.8-20
Flux		$L/m^2.h$	13-87	29-186
	COD	%	65-99	51-99
Rejection	TN	%	37-92	4-34
	TP	%	72-100	73-100
References				
			[244]	[245]
			[246]	[244]
			[247]	[246]
			[248]	[247]
			[249]	[249]
			[250]	[250]
			[251]	[252]
			[253]	[254]
			[203]	[255]
				[256]
				[253]
				[203]
				[257]

$$J_W = A * TMP \tag{5.3}$$

where J_w is the water flux in $(L/m^2.h)$, A is the water permeability coefficient in $L/m^2.h.bar$ and TMP is the transmembrane pressure in bar.

Equation 5.3 is then used to fit solute rejection which is a function of flux and solute permeability as presented in Equation 5.4.

$$\frac{1}{SR} = 1 + \frac{B}{J_w} \tag{5.4}$$

where SR is the solute rejection in %, and B is solute permeability in $L/m^2.h$.

The experimental solute rejection (SR) was determined using data on concentration of the solute in the influent (C_{infl}) and permeate (C_{perm}) as shown in Equation 5.5.

$$SR = 1 - \frac{C_{infl}}{C_{perm}} \tag{5.5}$$

Since the viscosity of the water changes with temperature, both J_w and SR were corrected for temperature known from the experimental data. The method used to correct for temperature is presented in Appendix C.1.1.

Water permeability (A) and solute permeability (B) are parameters that vary per membrane type (material and MWCO), type of influent and it's components [258, 259, 260]. Therefore A and B needed to be determined by estimating their values from experimental data [242]. Since in this study the solutes of interest are COD, TN, and TP, a solute permeability value B for each of these solutes needed to be estimated per membrane. For this, a normalisation method, implying the estimation of the normalised B values and re-scaling of these, was applied as described in Appendix C.1.2.

To estimate the water permeability value A per membrane, the fluxes and TMPs obtained from literature were fitted linearly using Equation 5.3. To estimate the B values, Equation 5.4 was implemented in MATLAB and solved with *fminsearch* which aimed to minimise the sum of squared errors between the model output and the experimental data available for each solute. A leave-one-out cross validation method, implying iterative model training and testing with the number of folds equal to the number of data points, was used to increase the estimation accuracy [261]. The quality of the predictions was evaluated via the root mean square error (RMSE, Equation 5.6) and the mean absolute percentage error (MAPE, Equation 5.7), where a MAPE lower than 10% means highly accurate prediction, $10-20\%$ means good prediction, between $20-50\%$ means reasonable prediction, and more 50% means inaccurate prediction [262].

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}-y)^2}{n}} \tag{5.6}$$

$$MAPE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{y-\hat{y}}{y} \right| \tag{5.7}$$

where n is the number of predicted data points, y is the data point and $\hat{y}$ is the predicted point.

Finally, the mean of all A and B values obtained with the training points was used in the optimisation model.

5.3.2 Optimisation model

Capital and operational expenditures (CAPEX and OPEX, respectively) are two of the most commonly used indicators in (waste)water industry [149]. These are often decisive for (large scale) implementation of membrane filtration [263]. Just like for any pressure driven membrane, the CAPEX of NF membranes is determined by the required membrane area to be purchased and installed. Often these costs account for all the auxiliary materials such as piping and pumps [264]. In this study CAPEX was considered to be the costs associated with purchasing and installing the membrane area required to treat the influent (A_{cost} is the cost in €/m^3 of influent) which was approximated as shown in Equation 5.8.

$$A_{cost} = \frac{Area * (\frac{P_{membrane}}{Lt_{membrane}} + \frac{INV_{cost}}{Lt_{installation}})}{Q * T} \tag{5.8}$$

where $Area$ is the total required membrane area in m^2 (equation is provided in Appendix C.1.3), $Lt_{membrane}$ is the membrane life time in years, in this study assuming this to be 5 years, $Lt_{installation}$ is the installation life time in years, in this study assuming this to be 15 years [265], P membrane is the price per m^2 of membrane in €/m^2, in this study assuming it to be 300 €/m^2 for both NF membranes [265], Q is the influent flowrate in m^3/h, T the operation time in $h/year$ and INV_{cost} is the investment costs in €/m^2.

The OPEX of membranes can be translated into water treatment costs which, for the nanofiltration of effluent from a wastewater treatment plant, can be considered to be mostly determined by the energy requirement per m^3 of treated water. Aspects like membrane replacement and labour requirements are very much dependent on the influent type and level of automation [264, 266]. The key variable selected and used in this study is TMP and the key responses are CAPEX and OPEX. The OPEX is associated with energy consumption which was approximated based on the pumping power required to ensure the desired TMP (equation is provided in Appendix C.1.3) [265, 267]. The pumping power was then used to approximate the energy costs (E_{cost} in €/m^3) of influent as shown in Equation 5.9.

$$E_{cost} = \frac{q * P_{energy}}{Q} \tag{5.9}$$

where, q is the pumping power in kW, P_{energy} is the price of energy in €/kWh, in this study assuming it to be 0.0941 €/kWh, valid for year 2019 [**?**], and Q is the influent flowrate in m^3/h.

The optimisation model finds the optimal membrane type (MWCO) and operational condition (TMP) to recover the targeted resources from a specific influent quality (characterised by COD, TN, and TP) and quantity (flow) while minimising the cost per $m^3$of treated water. The targeted resources were: water, COD, TN and TP. Depending on the targeted resource, the optimisation model indicated which membrane type and TMP should be chosen in order to optimise the quality and quantity of the recovered resources and associated membrane area (representing CAPEX) and energy requirements (representing OPEX). Thus the optimisation model, implemented and solved in MATLAB, looked at achieving the targeted water recovery and solute rejections while simultaneously minimising total costs per m^3 of treated influent. The method used for the optimisation is enumeration of all possibilities for flux and area by which to achieve the water recovery target. Then, from the solutions which simultaneously satisfy the water and the solute rejection targets (if set), the TMP and membrane type are chosen such that CAPEX and OPEX are minimised. In case the targets cannot be satisfied simultaneously, the model does not give a solution.

5.3.3 Sensitivity analysis

Depending on the geographical location of a wastewater treatment facility, seasonal demographic and climate aspects have an impact on the influent quality and quantity, which in turn are of great importance to the performance and thus design of a facility [268, 269, 270]. A few scenarios capturing the yearly fluctuations in influent quality and quantity and 100 random influent quality variations were used to evaluate the effect of changing influent quality and quantity on the model output (Table 5.2). This is meant to evaluate the sensitivity of the model in terms of membrane type selected to changing influent quality and quantity.

Furthermore, as mentioned earlier in this article, NF membranes are good at purifying water but also at separating mono- and polyvalent ions. Since the two NF membrane considered in this study perform differently, it is expected that a different membrane could be selected depending on the permeate targets. Therefore, the effects of the targets for the permeate quality and quantity on the model output were evaluated by changing these, while keeping the influent quality and quantity constant. For this, 1000 random variations of the targets were used to evaluate the sensitivity.

5.4 Results and discussion

5.4.1 Grey-box model

The mean values of all the estimated water (A) and solute permeabilities (B's), obtained through the leave-one-out cross validation method and the standard deviations, for the two membranes are presented in Table 5.3. The values of water permeability (the A's) are in accordance with the values found in literature for both membranes [259]. The standard deviations between the values obtained in training iteration (each fold) were 1.4% and 2.3% for NF90 and NF270, respectively. The values of COD, TN and TP permeabilities (the B's) were not found in literature. The standard deviations between the B's values obtained for both membranes in each training step were between 7.1% and 13.5%, greater than those of water permeability (the A's). This is mostly related to lack of consistency in the data used to estimate these parameters. The least consistent data set was for TN and TP rejections by NF270.

Table 5.2: *The scenarios used for sensitivity analysis of changing influent quality and quantity.*

Scenario	**Description**	**Calculation method**
BC	Yearly average concentrations and flow Q: 1 505 521 L/h COD: 40.38 mg/L TN: 8.58 mg/L TP: 0.48 mg/L	-
BC-Cs(+)	Increased concentrations, constant flow	Yearly average concentrations + 1.96 * $\frac{SD_c}{\sqrt{N_{DP}}}$
BC-Cs(-)	Decreased concentrations, constant flow	Yearly average concentrations - 1.96 * $\frac{SD_c}{\sqrt{N_{DP}}}$
BC-Q(+)	Constant concentrations, increased flow	Yearly average flow + 1.96 * $\frac{SD_Q}{\sqrt{N_{DP}}}$
BC-Q(-)	Constant concentrations, decreased flow	Yearly average flow - 1.96 * $\frac{SD_Q}{\sqrt{N_{DP}}}$
Random 100	Varying concentrations, constant flow COD range: 0-100 mg/L TN range: 0-40 mg/L TP range: 0-10 mg/L	-

SD_C=standard deviation in concentrations; SD_Q=standard deviation in flow; NDP=number of data points.

The predictions using the mean values of the estimated parameters are presented for NF90 in Figure 5.1 and for NF270 in Figure 5.2. The prediction qualities evaluated through MAPE show that the model performs well for most of the process variables, with MAPE values below 20% (Table 5.4). The predictions for TN rejections are the least accurate predictions per membrane, with an MAPE value of over 50% for membrane NF270. The prediction quality depends on (i) the specifications of the influent used for generating the data, (ii) the quality and quantity of the data used for parameter estimation, and (iii) the level of detail of the model used in this study (Equations 1 and 3). Membranes are selective to specific ions but in this study the exact concentrations of NH_4^+, NO_3^-, NO_2^- in the influent are neglected. The quality and quantity of the data can be a source of both systematic and random errors. A lack of model detail will mostly result in systematic errors, possibly even enhanced by the errors resulting from the data measurements. The modelling related systematic errors in this study could be related to not specifically accounting for example osmotic pressure of the influent, membrane fouling, concentration polarisation, membrane characteristics as surface change and zeta potential [271, 272].

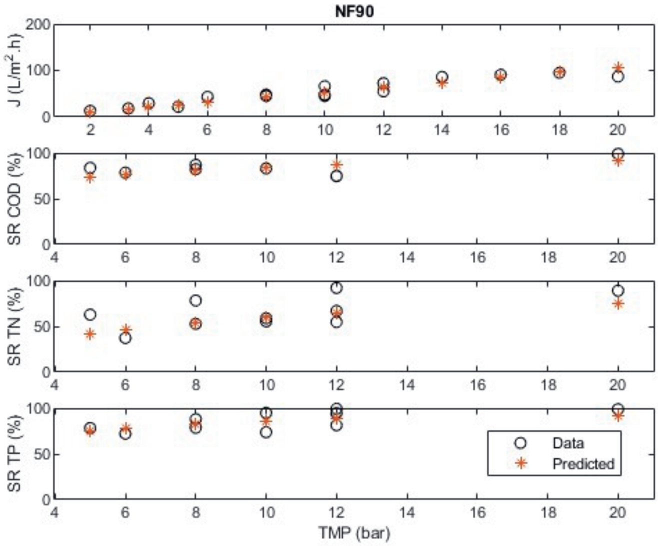

Figure 5.1: *Data and model prediction using the estimated parameters for the NF90 membrane.*

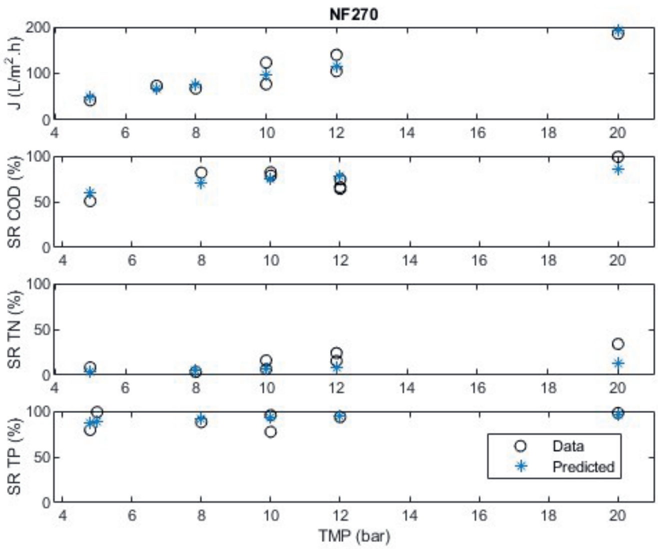

Figure 5.2: *Data and model prediction using the estimated parameters for the NF270 membrane.*

Table 5.3: *The mean estimated water (A) and solute permeability (B) values for NF90 and NF270 and the standard deviations.*

Parameter		Unit	NF90	NF270
	Mean	$L/m^2.h.bar$	5.32	9.68
A	SD	$L/m^2.h.bar$	0.08	0.22
	SD	%	1.4	2.3
	Mean	$L/m^2.h$	9.53	31.5
$\mathbf{B}_{COD}$	SD	$L/m^2.h$	0.91	2.23
	SD	%	9.3	7.1
	Mean	$L/m^2.h$	36.26	1251.10
$\mathbf{B}_{TN}$	SD	$L/m^2.h$	3.35	154.75
	SD	%	9.2	12.7
	Mean	$L/m^2.h$	8.75	6.47
$\mathbf{B}_{TP}$	SD	$L/m^2.h$	0.72	0.87
	SD	%	8.3	13.5

Table 5.4: *The root mean square error (RMSE) and mean absolute percentage error (MAPE) of prediction using the membrane model and the estimated parameters.*

	NF90		NF270	
	RMSE	MAPE	RMSE	MAPE
Jw	9 $L/m^2.h$	15%	16 $L/m^2.h$	15%
SR COD	7%	7%	10%	13%
SR TN	15%	17%	11%	51%
SR TP	8%	8%	8%	7%

5.4.2 Optimisation model

The optimisation model, minimising the costs per m^3 of produced water, was then run in MATLAB for the base case (BC). The required model inputs for the optimisation model were: influent quality, influent quantity, and targets for the permeate quality, depending on the desired water quality and recovery of resources. The model output consisted of the selected membrane and transmembrane pressure (TMP) as well as the achieved permeate quality, removal percentages, energy and area requirements with associated costs per m^3 of influent. The model input and output are presented in Table 5.5.

The performance ranges for both membranes were predicted between 4 and 24 bar using extrapolations which were 20% outside the range of empirical data found in literature. Both membranes showed a specific range of performance for the parameters of interest: flux and rejection of COD, TN and TP (Figure 5.3). From all possible options in this BC scenario, the optimisation model chose NF270 and a TMP of 8 bar (chosen point on Figure 5.3 and Figure 5.4) to recover 70% of the incoming water flow and to reach the targets for the permeate in terms of COD, TN and TP, while keeping the total costs (CAPEX and OPEX) as low as possible. The resulting flux was 77.4 $L/m^2.h$ and the required area was 15 654 m^2 resulting in a CAPEX of 0.18 €/m^3 of influent. This CAPEX was approximately 90% higher than the CAPEX for water reclamation with NF membranes reported by [219] and approximately 50% higher than the CAPEX for desalination with NF as a pre-treatment reported by [273], considering inflation. These higher cost estimates could be related to a combination of aspects which were different in this study such as cost per m^2 of membrane (incl. investment), shorter lifetime, differently quantified annual influent flow, etc. The OPEX, in this study determined by the TMP and flow, was 0.30 €/m^3 of influent, similar to the production costs for water reclamation via reverse osmosis membrane filtration reported by [235], considering inflation.

With the given 70% water recovery target for the BC, the NF270 membrane, in comparison with the NF90 membrane, is generally more advantageous for flux and thus for area requirements and total costs (Figure 5.4). Also, NF270 shows better performances in terms of TP removal but not in terms of COD and TN removal. Therefore, this membrane is likely to be chosen when water and TP recovery are a priority but the targets for COD and TN are not too stringent. The impact of different permeate targets is further evaluated in Section 5.4.3.

Table 5.5: *Optimisation model input and output for the base case (BC).*

Model input		**Unit**	**BC**
Influent	Q	L/h	1 505 521
	COD	mg/L	40.38
	TN	mg/L	8.58
	TP	mg/L	0.48
Targets for the permeate	Water	% recovery	70
	COD	mg/L (SR %)	$\leq$ 12 ($\geq$ 70)
	TN	mg/L (SR %)	$\geq$ 4 ($\leq$ 50)
	TP	mg/L (SR %)	$\leq$ 0.1 ($\geq$ 80)
Model output			
Selected	Membrane	-	NF270
	TMP	bar	8
Permeate	Flux	$L/m^2.h$	77.4
	COD	mg/L	11.68
	TN	mg/L	8.06
	TP	mg/L	0.04
Achieved solute rejection (SR)	COD	%	71
	TN	%	6
	TP	%	92
CAPEX and OPEX	Area	m^2	15 654
	A cost	€/m^3 of influent	0.18
	q	kW	478
	E cost	€/m^3 of influent	0.30

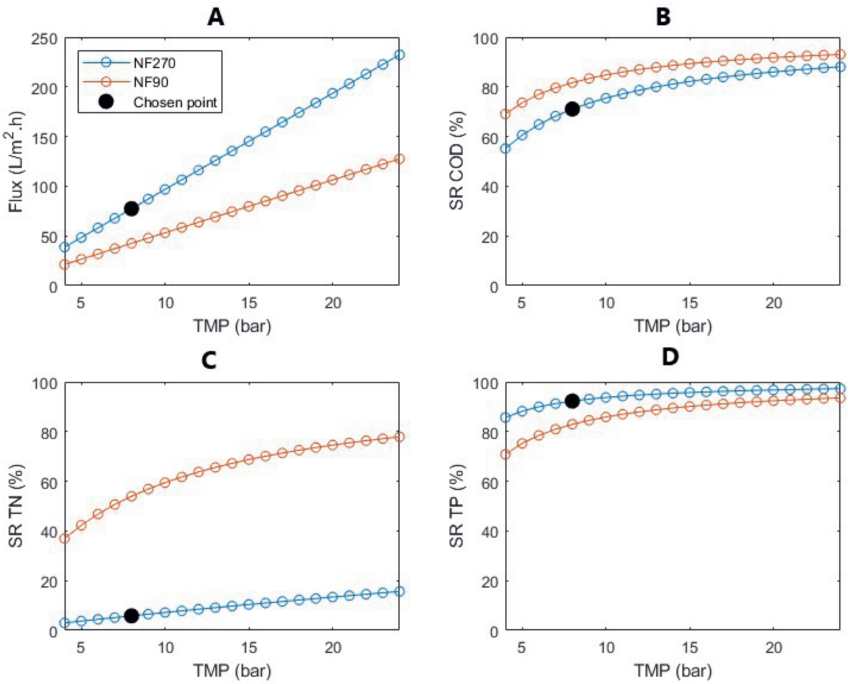

Figure 5.3: *The selected membrane and TMP (chosen point, black mark) from all possible choices with the two membranes (the empty marks) from 4 bar to 24 bar for flux (A), COD rejection (B), TN rejection (C), and TP rejection (D).*

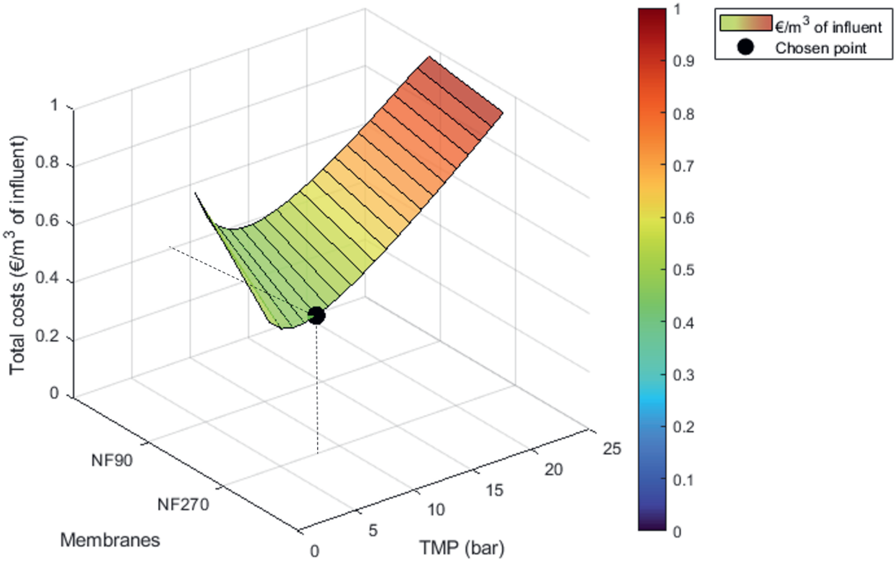

Figure 5.4: *The selected membrane and TMP (chosen point, black mark) from the range of total costs representing the sum of CAPEX and OPEX, both in €/m^3 of influent.*

5.4.3 Sensitivity analysis

Finally, a sensitivity analysis was carried out to evaluate the influence of the input parameters on the model output. The model outputs for the following changes were presented and discussed in this section: (i) influent quality and quantity, and (ii) targets for the permeate.

Influent quality and quantity

The effect of yearly fluctuations in influent quantity and quality were evaluated through a few scenarios with the annual 2.5%ile and 97.5%ile values for influent flow and concentrations of COD, TN, and TP from WWTP Walcheren, located in The Netherlands (approximately 150 000 PE treatment capacity; Table 5.2). The changes to the influent quality did not have an effect on the selected membrane, only on the selected TMP. This mostly because of the target set for TN recovery (≥ 4 mg/L) which in fact represented maximisation of TN passage through the membrane and NF270 retains less TN (Figure 5.3). The increase in the concentrations, potentially representing dry weather conditions, resulted in the selection of a higher TMP (9 bar, 1 bar higher than the BC). The decrease in influent concentrations, potentially representing rainy weather conditions, resulted in the selection of slightly lower TMP (7 bar, 1 bar lower than the BC). As the changes in the TMP were small, the changes in CAPEX and OPEX were minor as well: CAPEX between 0.16 and 0.21 €/m^3 of influent and OPEX between 0.26 and 0.34 €/m^3 of influent. Changes to the influent quantity (flow), potentially representing fluctuations in population, since the area of WWTP Walcheren is touristic, did not effect the choice of membrane and TMP. However, the surface area and energy requirement showed an increase or decrease with an increase or decrease in the influent flow, respectively. This was expected, since both the area and the energy calculations are flow-dependent. Therefore, fluctuations in flow might imply the requirement of buffers or that at times a certain number membrane modules would be redundant. Redundancy can be a positive aspect as it generally increases the flexibility of a process [149]. The results per scenario are presented in Table 5.6.

The model outputs for a water recovery target of 70% with randomised influent quality were presented in Table 5.7. From 100 random combinations of influent qualities, the optimisation model found feasible solutions for only 30 combinations. For the rest of the combinations no feasible solution was found to meet the targeted and fixed permeate quality. Of the 30 solutions found, NF90 was chosen only twice. The NF90 membrane was chosen for a rather specific influent:

Table 5.6: *The results for sensitivity analysis with yearly fluctuations in influent quality and quantity.Colour coding: blue-flux, yellow-achieved solute rejections, red-area and associated costs, green-energy and associated costs.*

			Unit	BC	BC-Cs(+)	BC-Cs(-)	BC-Q(+)	BC-Q(-)
Model input	Influent	Q	L/h	1 505 521	1 505 521	1 505 521	1 749 499	1 261 543
		COD	mg/L	40,38	43,83	36,93	40,38	40,38
		TN	mg/L	8,58	9,26	7,9	8,58	8,58
		P	mg/L	0,48	0,64	0,33	0,48	0,48
	Targets for the permeate	Water	%			70		
		COD	mg/L			≤ 12		
		TN	mg/L			≥ 4		
		TP	mg/L			≤ 0,1		
Model output	Selected	Membrane	-	NF270	NF270	NF270	NF270	NF270
		TMP	bar	8	9	7	8	8
	Permeate	Flux	L/m^2.h	77,4	87,1	67,7	77,4	77,4
		COD	mg/L	11,68	11,64	11,72	11,68	11,68
		TN	mg/L	8,08	8,66	7,49	8,08	8,08
		TP	mg/L	0,04	0,04	0,03	0,04	0,04
	Achieved solute rejection (SR)	COD	%	71	73	68	71	71
		TN	%	6	7	5	6	6
		TP	%	92	93	91	92	92
	CAPEX and OPEX	Area	m^2	15654	13915	17890	18191	13117
		A cost	€/m^3	0,18	0,16	0,21	0,18	0,18
		q	kW	478	538	418	555	400
		E cost	€/m^3	0,3	0,34	0,26	0,3	0,3

COD was 70 and 78 mg/L, TN was 26 and 17 mg/L, respectively, and TP was in both cases 0 mg/L. The combination of membrane type (NF90) and selected TMPs (9 and 10 bar) resulted in low energy requirements but the highest required area of all 30 solutions. The NF270 membrane was chosen for 28 of the 30 solutions, covering almost the full range of influent COD and TN, but only influent TP concentrations between 0-3 mg/L. For wastewater streams with phosphorus concentrations exceeding 3 mg/L the model did not find feasible solutions. The selected TMPs ranged between 6-24 bar. The area and energy requirements for the 28 solutions are according to the general trends presented in Figure 5.5. As TMP increases from 5 to 24 bars the energy requirement increases from 358 to 1433 kWh and thus the OPEX increased from 0.22 to 0.90 €/m^3 of influent. At the same time, the area requirement decreased from 20872 to 5218 m^2 and so did the CAPEX, from 0.24 to 0.06 €/m^3 of influent.

Table 5.7: *Model output for 100 random influent qualities within the provided ranges.*

		Parameter	Unit	Range			
Model input	Influent	Q	L/h	Base case			
		COD range	mg/L	0-100			
		TN range	mg/L	0-40			
		TP range	mg/L	0-10			
	Targets for the permeate	Water	% recovery	Base case			
		COD	mg/L				
		TN	mg/L				
		TP	mg/L				
Model output	Selected	Membrane	-	NF90			
		Times selected	-	2 out of 100			
		TMP	bar	9		10	
	Influent	COD	mg/L	70		78	
		TN	mg/L	26		17	
		TP	mg/L	0		0	
	Permeate quality	COD	mg/L	11.63		11.86	
		TN	mg/L	11.21		6.89	
		TP	mg/L	0.00		0.00	
	Achieved solute rejection (SR)	COD	%	83		85	
		TN	%	57		59	
		TP	%	85		86	
	CAPEX and OPEX	Area	m^2	25331.42		22798.28	
		A cost	€/m^3 of influent	0.29		0.26	
		q	kW	537.68		597.42	
		E cost	€/m^3 of influent	0.34		0.37	
	Selected	Membrane	-	NF270			
		Times selected	-	28 out of 100			
				Min.	Max.	Mean (calculated)	SD (±) (calculated)
		TMP	bar	6	24	13	5
	Influent	COD	mg/L	5	99	40.93	25.43
		TN	mg/L	5	40	22.00	12.01
		TP	mg/L	0	3	1.57	0.94
	Permeate quality	Flux	L/ m^2.h	31.9	127.6	69.1	
		COD	mg/L	1.00	11.83	7.88	3.74
		TN	mg/L	4.74	37.95	20.07	10.92
		TP	mg/L	0.00	0.10	0.07	0.03
	Achieved solute rejection (SR)	COD	%	65	88	78	8
		TN	%	4	16	9	3
		TP	%	90	97	94	2
	CAPEX and OPEX	Area	m^2	5218	20872	12431	5848
		A cost	€/m^3 of influent	0.06	0.24	0.14	0.07
		q	kW	358	1434	761	307
		E cost	€/m^3 of influent	0.22	0.90	0.48	0.19

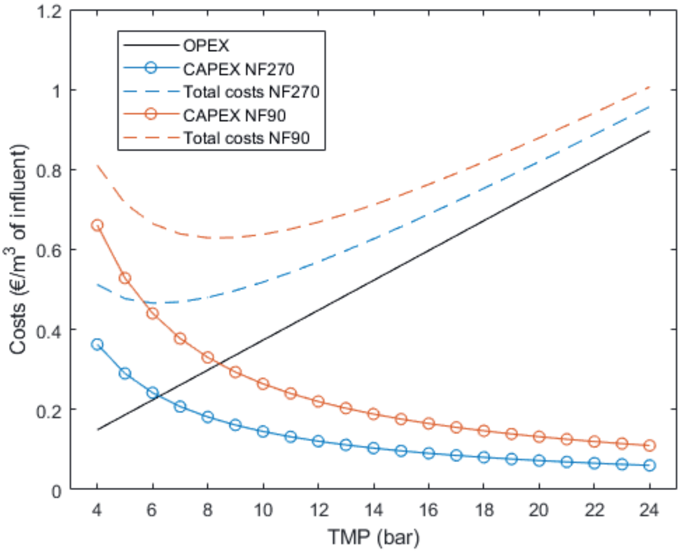

Figure 5.5: *CAPEX (area costs), OPEX (energy costs) and total costs varying with TMP for a water recovery target of* 70%*.*

Resource recovery targets

Next to variations in influent, the targeted permeate requirements were changed to evaluate how these affect the membranes chosen and the overall costs. For this 1000 random variations of all the permeate quality targets between 0% and 100% were tested with the same influent quality and quantity. The feasible model outputs for the 1000 random targets are presented in Figure 5.6. In the graphs A, B, and C, the height of the clusters on the y axis indicates that both membranes could achieve any water recovery target between 0% and 100%. The location of the clusters in the same graphs on the x axis represent the solutions space for COD, TN and TP targets. The trends in graphs D, E and F indicate that TMP determines the retention of COD, TN, and TP. This evaluation also visualises the infeasible regions for COD, TN and TP recovery (the blank spaces in each graph of Figure 5.6).

Overall, NF90 was the most selected membrane, 633 times while NF270 only 59 times. The NF270 was selected for a small range of low TN rejection targets (between 2%-16%) while NF90 was selected for a wider and higher TN rejection targets (between 44%-78%). While the choice for one of these two membrane is obvious in terms of water recovery and TN rejection, it is less obvious in terms

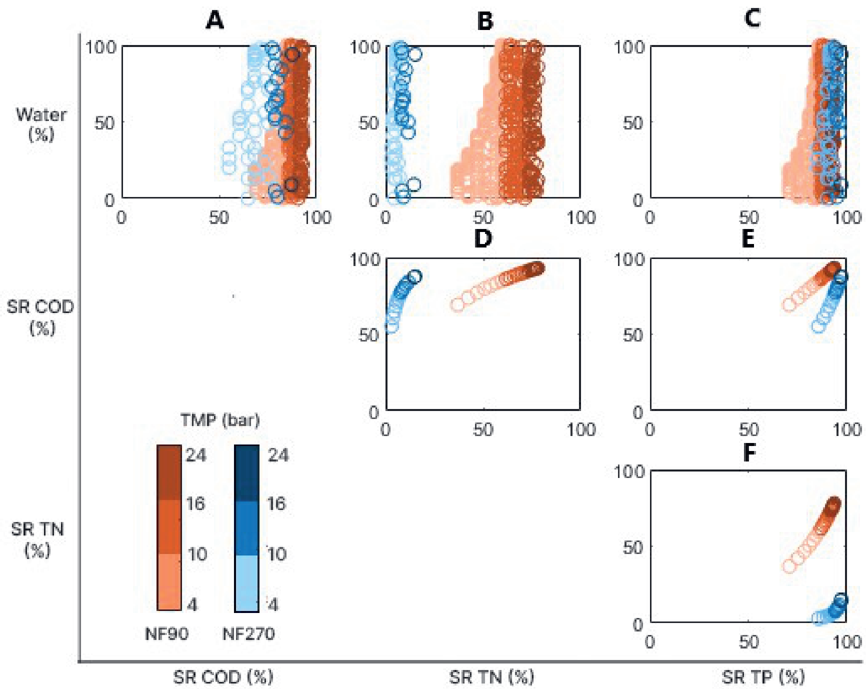

__Figure 5.6:__ The selected membranes and TMPs for different combinations of resource recovery targets.

of COD and TP rejection. The choice becomes even less obvious when more targets need to be met simultaneously and when different TMPs, as well as membranes with a more similar performance but differing costs are subject of choice. For example, when water recovery and TP rejection need to be simultaneously maximised (graph C), without setting any targets for TN or COD, both NF90 and NF270 are feasible solutions. Here a trade-off between the membrane surface area needed to maximise water recovery (determined by the membrane type) and the required energy (determined by the TMP) has to be made. Finally, the optimisation model was used to illustrate some of the most common scenarios related to permeate targets. The model outputs for these scenarios are presented and discussed in Appendix C.2. The result that stands out most is the scenario aiming to maximise water recovery without setting specific permeate quality targets (M-W, Table C.2.1 from Appendix C.2). The selected membrane was NF90 and the TMP was 12 bar. This is rather unexpected since NF270 better permeates water at even lower TMPs but the model still optimises for the best permeate quality at the lowest possible costs.

5.5 Conclusions

This study demonstrated that grey-box modelling of NF process performance ranges, that have a direct impact on cost, increases the accuracy of decision-making in the field of resource recovery from urban wastewater. Basic performance and cost optimisation of NF membranes can be achieved by modelling flux and solute rejections as a function of transmembrane pressure (TMP). For these variables (i.e. flux, solute rejection) empirical data is needed to estimate unknown parameters. The model accuracy is thus very much dependent on the quality of the empirical data. Nevertheless, a process model based on empirical data improves its applicability and therefore its relevance.

Depending on the resource recovery scenario (influent and targets), a different membrane type and/or the operating condition were more appropriate to minimise total costs. The results of this study showed that the selection of NF membranes (i.e. Dow NF90 or Dow NF270) and the operating conditions (i.e. TMP between 4-24 bar) is less dependent on the influent quality than on the targeted recovery performance. Yearly fluctuations in influent quality and quantity, resulted in the selection of the same membrane (NF270) and slightly different TMPs (7-9 bars). For more extreme variations in the influent quality the model selected primarily the same membrane (NF270), whereas the TMPs differed greatly (6-24 bar), almost the full range of TMPs covered in this study. When the targets for recovered water quality and quantity changed, the model selected different membranes and TMPs. This implies that the NF model used in this study is responsive to different resource recovery scenarios.

The application of the NF model for decision-making was demonstrated in a cost minimisation example. Such approaches can be reproduced for any other process and even extended to other economic, technical, environmental and/or social indicators. Safe reuse of recovered resource is key [190, 274]. Therefore, models should be able to predict also other relevant recovered resource quality indicators. For this [149] proposed two indicators that can also be used as constraints in a decision-making problem: risk of toxic compounds and risk of infection. To be able to qualify these two indicators, the NF model could be extended to predict rejections of, for example, heavy metals and bacteria or viruses. Moreover, the optimisation model implied the enumeration of all solutions simultaneously satisfying the targets. From those, the model selected the solution with the minimum total costs. However, considering the constantly increasing number of process available on the market, enumeration should be replaced with quicker multi-objective optimisation models such as goal programming [217].

Finally, decision-making for wastewater treatment infrastructure planning could benefit from a more extended knowledge library per processes, which include impact profiles of varying configurations and operational specifications. Doing so, the knowledge of operations can be incorporated into decision-making frameworks, thus increasing the reliability and understanding of the choices made.

6. Synthesis

6.1 Introduction

Resource recovery from urban wastewater can contribute to a more circular economy and ultimately to even communities' strategic autonomy [275]. However, the transition from wastewater treatment to resource recovery is increasingly complex. A growing number of processes, as well as economic, environmental, and social ambitions, are complicating the decision-making upon wastewater management practices. Simultaneously, developments in the computational field have proven to be able to deal with such complex problems and have been appreciated in the field of wastewater treatment. Computational tools and frameworks for decision-making for resource recovery have also been receiving increasing amount of attention [80]. The chapters of this thesis have highlighted, however, that the state of art knowledge in this field as represented in the literature is still incomplete and fragmented, and the work of this thesis aimed to fill some of the most apparent knowledge gaps, which is further elaborated on and discussed in this chapter.

The objectives as well as the main findings and conclusions per chapter are presented in Table 6.1. The contribution and limitations of the chapters are discussed in Section 6.2. Since interest in decision-making frameworks and tools has been growing, the limitations and added-values of a few simultaneous developments in the field are discussed in Section 6.3. Further on, the elements worth considering in future decision-making frameworks, mostly related to other recoverable resources and wastewater management trends, are elaborated on in Section 6.4. Finally, this chapter closes with a summary of or recommendations for future research and development in Section 6.5.

6.2 Research contribution and limitations

6.2.1 Quantitative evaluation, even of qualitative aspects

In this thesis, key performance indicators (KPIs) belonging to technical, environmental, economic, and social criteria, were defined and mathematically formulated to serve the evaluation and design of resource recovery from urban wastewater (Chapter 2). The mathematical formulations implied quantification of the indicators, even of indicators of qualitative nature. To quantify qualitative KPIs, like odour emission potential and acceptability, certain aspects (i.e. odour emission potential per process and degree of human contact) were linearly discretised, so that process (i.e. physical, chemical, biological, thermal) and resource types

Table 6.1: *Overview of the research chapters with the objective, main findings, and conclusions per chapter.*

Chapter	Objective	Main findings and conclusions
Chapter 2 KPIs for evaluation and design	This study proposed mathematical formulations for a set of accessible key performance indicators (KPIs) to support the delivery of evidence to both private and public decision-makers about the benefits of resource recovery options and help them to mitigate potential risks.	For model-based design of treatment trains: • indicators need to incorporate process, context, resource, and legal characteristics; • social and environmental constraints are critical as they ensure the viability of treatment trains. For both model-based evaluation and design of treatment trains: • it is important to align information from technology suppliers with local, national, or international regulations for wastewater treatment and resource reuse.
Chapter 3 Model-based design - conceptual framework	This study presented a framework for model-based design of treatment trains that can simultaneously recover water, energy, and/or nutrients (i.e. nitrogen, phosphorous) from urban wastewater using a weighted multi-objective multi-integer non-linear programming (WMOMINLP).	• Grouping unit processes based on the minimum required and maximum allowed COD levels ensures fast optimisation so the groups determine the order of the processes • The model does not (yet) provide the exact location of unit processes within a group; to provide the exact location of unit processes, heuristics with logic ('if-then') rules from experts are required. • The optimal solution for a given scenario is very much dependent on (i) the consistency of the information per unit process in the knowledge library and (ii) the evaluation criteria chosen by the user.
Chapter 4 Existing versus new plant configurations	This study evaluated the trade-offs (i.e. technical, economic, environmental, and social) between new and existing conventional configurations for resource recovery and the sensitivity of the results to yearly influent variation, plant size, and criteria weighting.	• The results were only sensitive to plant size (i.e. small, medium, and large scale) and criteria weights but not to influent variations. • At small scale new and at large scale the existing plant configurations ranked best. • An increase in the weight assigned to the economic criterion results in higher ranks for the existing configurations, while an increase in weight assigned to the environmental criterion results in higher ranks for the new configurations. • The sensitivity to scale highlights the importance of accounting for influent flow rates in the quantification of KPIs. • The sensitivity to weights highlights the role of multi-criteria in deciding upon the recovery of resources from urban wastewater.
Chapter 5 Model-based decision-making at process level	This study demonstrated how the inclusion of more details (in this case, configuration and operational settings) of a single process for resource recovery influences the decision-making at process level.	• Basic performance and cost optimisation of NF membranes can be achieved by modelling flux and solute rejections as a function of transmembrane pressure (TMP). • Recovery targets determine the selected membrane type and operating pressure. • Seasonal influent fluctuations affected only the selected operating pressure. • Thus, the model in this study is robust where needed and responsive to different resource recovery scenarios when required.

(i.e. energy, nutrients, irrigation water, industrial water, and drinking water) were graded with linearly increasing or decreasing integers. The linear aspect of the discretisation, although widely applied, is of course debatable [276] and thus could be subject to further research. Thus, despite this approach enabling systematic design (Chapter 3) and consistent comparison of treatment trains (Chapter 4), it would need to be validated, separately, by experts in the field, resource end-users, and policymakers. This would be the next step in bringing the DST framework to implementation and use in practice.

For decision-making, both quantitative and qualitative assessments can be used. Quantitative assessments are preferred over qualitative ones as they reduce the interpretability of the indicators and enable the use of weights [277]. However, quantifications are very much data quality and quantity dependent [34]. The quantification methods in this research contained generalised values for several parameters which can vary with and even within the context (context-generic approach). Several KPIs, in particular social ones, like affordability and acceptability are related to a specific case and the population served. Thus, alternatively, such indicators could be assessed qualitatively, inquiring the decision-maker to provide this information about the population served as an input through a user interface/dashboard of the decision support tool (Chapter 3). This input, however, needs to be discretised again so that it can be used for evaluations and that, eventually, results can be presented in some quantitative form (ranking, graphs, tables) for objective comparison in that given context. Introducing this feature could make the current framework more context-specific.

6.2.2 Feasibility goes beyond compatibility

The framework presented in Chapter 3 is not (yet) able to identify the most feasible resource to be recovered from a specific influent. Currently, the framework described in the research presented here requires the decision-maker to decide what resource(s) to recover. The conceptual framework is then able to automatically choose compatible unit processes to recover the desired resource(s) (i.e. water, energy, nitrogen, and/or phosphorous) based on given process constraints, e.g. the minimum required and maximum allowed COD levels. Thus the framework chooses unit processes that can handle the COD concentration of the stream entering the unit processes. The framework selects as many unit processes as needed to comply with regulation (i.e. effluent quality compliance) and safety constraints (i.e. risk of infection and risk of toxic compounds). Then, it optimises the selected compatible processes for other technical, economic, environmental, and social indicators. The constraints and indicators, as defined in Chapter 2, accounted for context-related aspects like local regulation, climate change awareness, and net average income. Therefore, the framework generates treatment trains feasible for the context in which they would be placed to recover the predefined resources.

Furthermore, as demonstrated in Chapter 4, the KPIs as defined in Chapter 2 are sensitive to the scale of implementation. However, the framework has not been built to identify scale-related feasibility such as, for example, which resource should be recovered at what scale. To find which resource is feasible to recover at several scales with the current framework, the decision-maker would need to take the steps listed in Figure 6.1.

The described Full Factorial Design of Experiments with the varying factors 'scale' and 'resource' will eventually help identify the optimum scale and treatment train per recoverable resource. But even then, the combinations of scales are not yet taken into account, for example, water recovery can be feasible at a local and decentralised scale (i.e. household or neighbourhood level), whereas energy and nutrient recovery may require collection at a centralised location (i.e. city or regional level). To find the optimal treatment train per resource, the interdependency of treatment trains needs to be built into the model. Also, such evaluations should have extended system boundaries including transportation (i.e. piping, truck drives) with associated economic, environmental, and social impacts [278]. This level of complexity introduces the need to include even more heuristic inputs in the decision-making process [187].

6.2.3 Pollution control and resource recovery

The main task of existing wastewater treatment is pollution control. At no time should pollution control be compromised with resource recovery from wastewater. In fact, in the case of resource recovery, not only the quality of the effluent but also of the recovered resources needs to comply with regulations. Effluent standards are limited to a few key parameters, most often including COD or BOD, TN, TP, and/or specific nitrogen and phosphorus species [279]. These were used in the developed framework. However, for resource reuse more specific regulation and thus evaluation and design of candidate scenarios is needed.

While pathogens and heavy metals are of greatest concern for humans and the environment, mostly due to their high concentration in the influent, chemical and organic micropollutants are considered to pose risks for human health and the environment in the long term [280, 102]. In this sense, the framework in Chapter 3 accounts for heavy metals and pathogens in the effluent and recovered resources

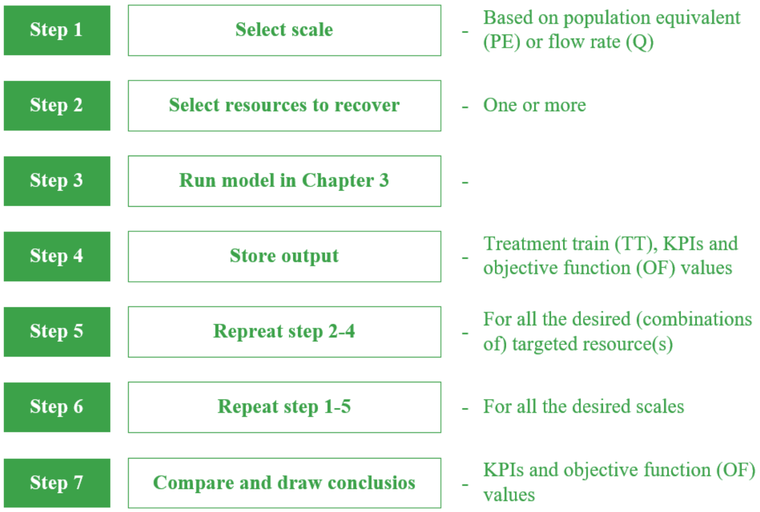

Figure 6.1: *The sequence of steps to be taken with the current framework for exploring the recovery of different (combinations of) resources at various scales.*

in the form of constraints related to the risk of toxic compounds and the risk of infection, respectively. To increase the reliability of evaluation and design models in the long run, the risk of toxic compounds should also include chemical and organic micropollutants such as pharmaceutically active compounds (PhACs), personal care products (PPCPs), and hormones [281, 91]. These need to be accounted for so that the tool can select additional processes if needed. Additional treatment may, however, have adverse effects in terms of, for example, new toxic compounds, more contaminated sludge, energy consumption, and greenhouse gas emission [280, 279]. Nevertheless, for a technology to be considered as a candidate in decision-making tools, technology suppliers need to report on the removal of all the pollutants relevant for the final resource to be recovered, which is not the case today. An option to deal with this is to choose the most recalcitrant pollutants as indicator compounds for sets of pollutants [93, 282, 283].

6.2.4 Process modelling to improve the model-based evaluation and design of treatment trains

Currently, both the framework in Chapter 3 and the evaluation in Chapter 4 are relying on one single performance per process per component (i.e. water, COD, TN, TP, heavy metal, pathogens). However, unit processes are known to perform differently, depending on the type of influent, specific configuration of the unit, and operating conditions. Therefore, Chapter 5 of this thesis explored the possibility and relevance of increasing the level of detail per process in terms of performance, depending on configuration and operational details, and the associated effect on costs. For this, in Chapter 5 a grey-box model for nanofiltration was used to predict COD, TN, and TP rejection as a function of transmembrane pressure for two different membrane types in molecular weight cut-off. The results demonstrated that a given process can be operated differently to meet resource recovery targets. This is of relevance to the reliability of the framework presented in Chapter 3 which chooses processes based on their performance. The approach presented in Chapter 5 can be applied to any other process known to have a range of performance, especially concerning the recoverable resources (i.e. water, COD, TN, and TP). However, before applying the grey-box modelling approach presented in Chapter 5 to other processes, a comparison with white- and black-box modelling approaches in terms of model reliability, computational speed, required memory, etc. may help to choose the right level of complexity within the decision framework.

6.2.5 Supporting the transition from wastewater treatment to resource recovery

Converting WWTPs into water, energy, or other resource recovery plants (RRPs) requires adequate infrastructure and well-established logistic networks [284, 204]. This implies the need for policy, legislation as well as economic incentives to support the recovery and reuse of resources but also to limit the exploitation of non-renewable resources [285, 286]. There is a wide range of activities that can be carried out by responsible organisations at a local, regional and national level, from legal frameworks supporting the handling of resource-containing streams to rewarding sustainable resources [287].

The proposed KPIs in Chapter 2 and the model in Chapter 4 can be used to evaluate the potential in terms of quality and quantity of the recovered resource and the associated economic, environmental and social implications. However, to understand the implications of widely implemented resource recovery, treatment trains should be evaluated from a regional, national, and ultimately global perspectives. For this, as mentioned earlier in this chapter, the system boundaries would have to be extended, extended potential risk evaluations and maybe the integration of lifecycle costs (LCC) and lifecycle analysis (LCA) tools might be needed.

6.3 Simultaneous developments in the field

A few latest developments in the field (tools and frameworks for resource recovery from urban wastewater), other than those already mentioned throughout the chapters of this thesis have been listed in Table 6.2. The tools and frameworks considering multiple resource recovery either (i) focus solely on the recovery of those resources, without considering wastewater treatment [288], (ii) provide the framework in terms of steps to be taken for decision-making, without providing a mathematical model [34], or (iii) generate treatment trains manually, without a model [62]. [289] provides the mathematical model for generating trains only for the recovery of energy. One promising tool would be the NOVEDARplus_EDSS tool [48], however, no articles or reports have been published about this tool yet.

Given the aspects considered and methods used in the tools and frameworks listed in Table 6.2, this thesis remains unique by (i) proposing a model for the evaluation and design of treatment trains for wastewater treatment and multi-resource recovery, and by (ii) addressing ways to improve this model. Nevertheless, these tools and frameworks have elements that are worth adopting in the model present in this thesis. These aspects include recovery of other resources, accounting for regional aspects, generating more than one treatment train as output, and accounting for regional aspects. Most of these elements are further elaborated on in the following sections.

6.4 Outlook

The research described in this thesis focused on the recovery of water, chemical energy (COD), nitrogen (TN), and phosphorous (TP). These studies only considered the treatment and recovery of these resources from centralised conventional urban wastewater. There are, however, other interesting resources to be recovered and other wastewater management trends, which have not (yet) been taken into account. In the following sections, other commonly recovered resources and wastewater management trends are presented, along with the possibilities and challenges of incorporating these into the model presented in this thesis.

Table 6.2: *Simultaneous developments in the field.*

Tool/framework	Description	Resources	Publications or reporting	Reference	Considerations for future research
WOW! Interreg North-West Europe decision support tool (WOW! DST)	Evaluating the suitability of an existing wastewater treatment plant for the recovery of any carbon-based materials	Bioplastics (PHA), lipids, and cellulose	DST in Excel is available on the project webpage	[288]	The recovery of carbon-based resources
Framework for planning and implementation of resource recovery at urban wastewater treatment plants in mega cities	Proposing a sequence of steps to identify the resources and the technologies for recovery at a given location	Water, biofuel, heat, nutrients, soil conditioner, organic matter.	Article but no model	[34]	Accounting for regional aspects like the legal and regulatory framework in place and the relevant stakeholders for partnership and institutional arrangements
Tool for early-stage design and retrofitting of wastewater treatment plants	Generates plant layouts based on influent characteristics, effluent constraints, and objectives (three KPIs).	Energy	Article with optimisation model provided in supplementary material	[289]	More than one treatment train as an output
Decision support system (DSS) for the implementation of energy recovery from sewage sludge	Pair-wise comparison of all possible combinations (manually generated) of five processes using a set of KPIs	Thermal and chemical energy	Article but no model	[62]	Accounting for regional aspects like material circularity index
NOVEDARplus_-EDSS (extension of NOVEDAR_EDSS)	3R' concept where the Rs stand for reduce, reuse, and recover.	Water, nutrients, and other organic valuable products such as biopolymers and bioplastics	None yet	[48]	The reuses of recovered resources

6.4.1 Other resources

Thermal energy (heat)

Urban wastewater, depending on the geographical location, distance from the discharge point, time of the day, and the season, may have temperatures ranging on average between 2-25 °C [290, 291, 85, 292]. According to [86], 1°C extracted from 1 m^3 for wastewater is equivalent to 1.16 kWh. This thermal energy can be extracted at various locations, starting from the source (i.e. household, building), along the sewer, and the WWTP [85].

Research and practice have demonstrated that wastewaters with temperatures above 10 °C and flows above 50 m^3/h are interesting for heat recovery [86]. As it implies cooling of the stream used, heat recovery from the raw influent can have an impact on the nitrification (nitrogen removal) capacity of activated sludge plants, which generally requires temperatures between 8-10 °C [293]. Moreover, heat recovery from raw influent can be technically challenging due to fouling of heat exchangers and fluctuating flows and temperatures [85]. Heat recovery from the effluent, which is stable in terms of quality and quantity, is more beneficial for heat exchangers [290, 293]. According to [294] thermal energy recovery (heat) from tertiary treated effluent through a water source heat pump (SWHP) could contribute for approximately 40% to a "net-zero" LCA-based impact and improved total environmental impact.

Recovered heat could be used in various ways including redistribution to districts or industry. However, when heat distribution facilities are not available or the price the end-user is willing to pay is too low [56], recovered heat could best be used at the treatment train level. Thus, for proper decision-making regarding heat recovery, the heat demand and monetary aspects should be included [5].

Carbon (cellulose, biopolymers, etc.)

In the western culture, 30-50 % of the suspended solids and 20-30 % of the total COD in the raw urban wastewater influent is cellulose from toilet paper [295, 296]. Fractions of cellulose can also be found in the primary, return, and excess sludge of conventional activate sludge processes [48, 87]. Cellulose in wastewater represents slowly degradable COD and thus its removal can increase the efficiency of wastewater treatment plants [295]. Furthermore, cellulose can be recovered from influent as well as from sewage sludge and be reused as a source of COD for biological water treatment [297] or as a raw material for various industries including construction materials [87, 298], the production of VFAs as a precursor for other products [299, 300], and even for production of nanocellulose as a high-grade bio-material which is still under research and development [301]. Cellulose can be recovered from wastewater raw influent via fine-mesh screens or sieves [302, 296]. However, depending on the valorisation intentions of the recovered cellulose and the legal frameworks in place (i.e. end-of-waste status), additional downstream processes should be accounted for by decision-support tools for resource recovery from wastewater.

Overall, urban wastewater is rich in low-value carbon which can be upgraded to extracellular polymeric substances (EPS), more specifically polyhydroxyalkanoates (PHA) and alginate-like-exopolymers (ALE), as raw materials for diverse industries including agriculture and construction materials [303, 198, 304]. EPS produced from wastewater can be harvested from excess sludge of conventional activated sludge but also membrane bioreactor processes and reused in the (waste) water industry for coagulation-flocculation [305]. PHAs can be efficiently and economically produced from urban wastewater [306, 84] by excess activated sludge under specific conditions including alternative aerobic-anaerobic conditions, C: N ratio, pH, and sludge retention time (SRT) [307]. Most commonly fermented organics (VFAs) obtained through partial anaerobic digestion are used as a soluble carbon source to enhance the PHA production which then comes at the expense of biogas production [303]. In fact, VFAs from wastewater can also be seen as a renewable resource, a raw material for many industries including pesticides and paints [300].

Potassium

Potassium (K) is one of the three macronutrients, N, P, and K, required for agriculture in comparable, actually slightly higher quantities than phosphorus [19]. This primary nutrient is currently being mined and the natural reserves of potassium (potash) could run out even faster than the phosphorus reserves [83]. Although potassium is available in urban wastewater [308], its recovery has received insignificant attention in comparison with phosphorus. Potassium enters the wastewater mostly via feces and urine [91]. In conventional wastewater treatment plants, potassium accumulates in sludge and most commonly ends up in the centrate and it can be recovered in the form of potassium struvite (magnesium potassium phosphate, MPP) as an alternative to ammonium struvite (magnesium ammonium phosphate, MAP) [48, 83]. However, potassium recovery in the form of potassium struvite can be hindered by the presence of nitrogen, thus nitrogen should be removed prior to potassium struvite recovery [309]. Nitrogen could be removed either through ammonia stripping or ANAMMOX processes. Alternatively, potassium but also other ions, such as sodium, can also be recovered through capacitive deionisation (CDI), a rather novel process able to selectively separate specific ions based on their valence [310].

6.4.2 Other trends

Source-separated sewage streams

Resources can also be recovered from source-separated streams like grey-, black- and/or yellow-water [311, 7]. Source separation of urban wastewater implies the separation of water, COD, TN, and/or TP as well as of other pollutants as presented in Table 6.3, and this means that resource recovery can be done more efficiently [312]. Besides this, source separation has also the benefit of reduced or specific contamination of streams [281, 313], with most heavy metals, pathogens, and some pharmaceuticals in black-water and or yellow-water and most personal care products in grey water (Table 6.3). This enables targeted removal of pollutants and treatment of the individual streams. This could increase the acceptance of a resource, e.g. if water is recovered from grey water. However, for the design and evaluation model to account for source-separated streams, it would need to generate several treatment trains and maybe even interconnect them by adding the effluent of one stream (treated black- and yellow-water) to the treatment train of another stream (grey-water). This only makes sense if it improves the overall rating of the entire system, especially when considering the distribution of micropollutants in the streams.

Decentralisation

Conventional urban wastewater management implies central water treatment, distribution to end-users (i.e. households, agriculture, industry, etc.), and then collection of used water (i.e. wastewater) and treatment in central wastewater treatment plants. An alternative to this is decentralisation of wastewater treatment and local reuse. This alternative water and wastewater management practice, for both treatment and resource recovery, has been advocated by many for decades already as a more sustainable option, in various contexts (i.e. socio-geographical and economic) [220, 315, 316, 222, 317]. The benefits of decentralisation of resource recovery vary depending on aspects such as the context in question (i.e. location, legislation in place, etc.), processes for treatment and recovery, the specific resources to be recovered, and the degree of source separation of streams [318]. The presented framework in Chapter 3 also allows evaluations at smaller scales, however, not when streams are separated at the source. In that case, the framework would require adjustments as described in Section 6.2.

6.5 Recommendations for future research and developments

Firstly, to maximise the reliability of a design framework or tool for resource recovery from urban wastewater, the used process performance should be as realistic as possible. Therefore, it is recommended to carry out further research comparing various degrees of details for process modelling in varying process conditions using existing experimental data. Currently we are investigating the comparison of several white, grey- and black-box models for predicting phosphorus recovery rates in struvite reactors. Future research should also evaluate if and how the process models themselves and their responses impact the quality of the output and the efficiency (i.e. computational speed and required storage capacity) of the design framework or tool.

As the number of candidate processes for resource recovery increases and the decision-making system boundaries are broadened, the complexity and thus the non-linearity of the problem is expected to increase as well. To address this

Table 6.3: *The percentage of water, COD, TN, and TP content of conventional urban wastewater in source-separated streams according to [91, 314]; the heavy metal, organic, and chemical (micro)pollutant distribution over the streams according to [281, 313].*

Streams	**Sub-streams**	**Content** **Water, COD, TN, TP**	**(Micro)pollutants**
Conventional urban wastewater		C_{COD} : 210740g/m^3 C_{TN} : 2080g/m^3 C_{TP} : 423g/m^3	Heavy metals (dietary and non-dietary origin) Human hormones Pharmaceuticals Personal care products
Source separated streams		**% of conventional urban wastewater**	**Distribution (majority)**
Black-water	Urine (yellow-water)	1% of Water 10 % of COD 76 % of TN 45 % of TP	Heavy metals (mostly of dietary origin) Human hormones Pharmaceuticals
	Faeces and toilet paper	29% of Water 46 % of COD 14 % of TN 32 % of TP	
Grey-water	Shower, bathtub, kitchen sink, dishwasher, laundry.	70 % of Water 44 % of COD 10 % of TN 23 % of TP	Heavy metals (non-dietary origin) Personal care products

problem, extensive comparative research should be carried out to identify the best/most suitable optimisation methods as an alternative to weighted multi-objective mixed-integer non-linear programming. The aspects to be considered in such comparative research should be mainly related to the quality of the output and the efficiency of the methods, with specific attention to the quality of the output which tends to be compromised by computationally less expensive methods and models [276].

Furthermore, the possibility and benefits of integrating specific tools for extending the system boundaries of the framework presented in this thesis should be researched. For example, life cycle costing (LCC) and life cycle analysis (LCA) could replace the current economic and environmental indicators, respectively, presented in Chapter 2 of this thesis [319]. For extending the spatial boundaries of resource recovery decision-making frameworks, Geographical Information System (GIS) could greatly contribute to increasing the reliability of the model or framework outputs, especially when resource reuse is accounted for [137]. Integrating GIS in resource recovery decision-making frameworks could potentially help in decoupled resource recovery evaluations to identify which resource could best be recovered at what scale (i.e. local, regional, national) considering supply and demand hotspots [278, 22, 320, 321, 322, 323]. These tools have been previously employed in individual, case-specific studies but not in decision support tools or systems for the design and evaluation of multi-resource recovery from urban wastewater. The integration of such tools could contribute to future-proof decision-making, very much needed in the midst of climate change and geopolitical conflicts threatening resource availability, environmental quality, and social well-being [24].

The topic of this thesis can be considered to be of multi-scale complexity (Figure 6.2). To evaluate and design treatment trains, it was needed to account for the removals of components, the performance of unit processes, and the aspects of the local context such as the demand-supply ratio of resources. In this thesis, the local context has been accounted for through the KPIs, however only briefly. The wide implementation of resource recovery from urban wastewater would require models to consider the local and regional energy, water (natural -surface and ground- and anthropogenic), and other relevant resource or management systems and networks such as the financial networks. Therefore future research could best focus on finding ways to integrate models of relevant systems and networks.

Finally, as explained by [276], to develop digital tools for such complex problems, any single "expert" can be considered a "rookie" mastering only parts of the problem. Thus the involvement of experts and stakeholders from various disciplines is needed. Experts and stakeholders could be involved in the engineering but also a validation of the entire decision-making framework.

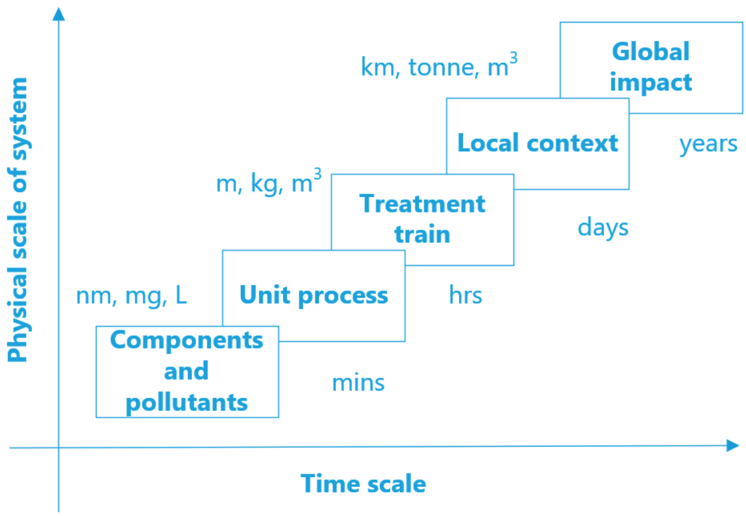

Figure 6.2: *The multi-scale complexity of decision-making for resource recovery from urban wastewater, adapted from [276].*

APPENDIX A. SUPPORTING MATERIAL FOR CHAPTER 2

A.1 Abbreviations

Abbreviations	Unit	Description
UP	-	Unit Process
TT	-	Treatment train
TT_k	-	Treatment train involved in recovering compound k
A_j	m^2/m^3	Surface area required for UP j
$Acceptability_{TT}$	-	Acceptability of the whole TT
$Affordability_{TT}$	-	Affordability of the whole TT
$CAPEX_j$	€	Capital expenditure of the UP j
$CAPEX_{TT}$	€	Total capital expenditure for whole TT
CCA_c	%	Percentage of people aware of climate change per country c
CCT_c	%	Percentage of people perceiving climate change as a threat per country c
$Cpe_{i,k}$	cfu/100ml	Limit concentration of pathogen i equivalent to 10^{-6} DALYS pppy for resource k
D_{TT}	days	Number of days of operation of TT
$DS_{k,c}$	-	Demand supply ratio of resource k in country c
EAC_j	€/year	Equivalent annual cost for UP j
EAC_{TT}	€/year	Equivalent annual cost for the whole TT
$EQCI_{TT}$	binary (0-1)	Effluent quality compliance index for the whole TT
FC_{ik}	mg/L	Final concentration of compound i in recovered resource k
$Flex_{TT}$	-	Flexibility of the whole TT
FP_{TT}	m^2	Land footprint of the whole TT
$fr_j(p)$	%	Failure rate of UP j in specific time period
H_{TT}	hours	Number of hours of operation per day for the TT
HC_k	Scale 1-5	Degree of human contact per recovered resource k
HRT_j	hours	Hydraulic retention time per UP j
IC_i	mg/l	Initial concentration of compound i in the influent of the TT
$Infl_{COD,j}$	mg/l	Concentration of the COD in the influent of the UP j
$LC_{i,l,k,c}$	mg/l	Limit concentration for compound i per location l per resource k per country c
LNP_j	dB	Level of noise potential per unit process in dB
$LR_{i,j}$	log scale	Log reduction of compound i by unit process j
Lt_j	years	Life time per UP j
$max_{v,j}; min_{v,j}$	-	Minimum required and maximum allowed value for the variable v per UP j
NAI_c	€/pppy	Net average income per person per year in country c
NEP_{TT}	dB	Noise emission potential by the whole TT

continued on the next page

Abbreviations	**Unit**	**Description**
OEP_j	-	Odour emission potential by unit process j
OEP_{TT}	-	Odour emission potential by the whole TT
OP_j	scale 1-4	Odour potential per type of process
$OPEX_j$	€/year	Operational expenditure of the UP j
$OPEX_{TT}$	€/year	Total operational expenditure for whole TT
$or_{v,j}$	-	Operating range for variable v of UP j
PE	people	Population equivalent
PI_i	binary (0-1)	Pollution index for compound i
PI_{TT_k}	-	Total pollution index of TT for recovered resource k
PIG_k	€/year	Potential income generated by the recovery resource k
PIG_{TT}	€/year	Potential income generated by the whole TT
pppy	-	per person per year
$Q_{influent}$	m^3/hour	TT influent flow rate
r	%	Yearly discount rate (depreciation rate)
$R_{j,k}$	%	Percentage of compound k that goes to the side stream in UP j
$range_{v,j}$	-	Operating range per variable v of UP j
$RatioInfection_{TT_k}$	-	Perceived potential risk of contamination with pathogens
$RatioToxic_{TT_k}$	-	Perceived potential risk of contamination with toxic compounds
Rel_{TT}	%	Reliability of the whole TT
RI_{TT}	binary (0-1)	Risk of infection for the whole TT
$RLR_{i,k}$	log scale	Required log reduction of pathogen i per recovered resource k
RTC_{TT}	binary (0-1)	Risk of toxic compound for the whole TT
TLR_{i,TT_k}	log scale	Total log reduction of pathogen i achieved via TT for the resource k
$VRP_{k,c}$	€/m^3, €/kg	Value of the recovered resource k in country c
WTP_{TT}	-	Willingness to pay for the environment for whole TT
X_k	kg/hr, m^3/hr	The (mass) flow rate of recovered resource k
$Y_{j,k}$	%	Removal/recovery % of compound k by UP j, for the main/side stream
Mathematical symbols		
$\in$	-	Is member of
$\forall$	-	For all
$\sum$	-	Sum
$\prod$	-	Product

A.2 Literature review

Table A.1: *Categories of indicators used in literature for the evaluation of urban wastewater treatment and/or resource recovery, the type of definition provided and the indicator selection method applied. E=energy recovery, P=phosphorous recovery, N=nitrogen recovery, Eff=effluent quality, Eco=economic, Env=environmental, Soc=social, Tec=technical. + means that the reference covers the topic or it includes the category of indicators; - means that the reference does not cover the topic or it does not include the category of indicators.*

Reference	Topic covered					Categories of indicators				Definition	Selection method
	E	P	N	W	Eff	Eco	Env	Soc	Tec		
[104]	+	+	+	+	+	+	+	+	+	Phrased	Literature review
[99]	+	+	-	+	-	+	+	+	+	Phrased	Literature review, Stakeholder engagement
[324]	-	-	-	-	+	-	-	-	+	Mathematical	None
[101]	-	-	-	-	+	+	+	+	-	Phrased	Author's opinion
[325]	-	-	-	+	-	+	+	+	+	None	Literature review
[105]	+	+	+	+	+	+	+	+	+	Phrased	Literature review
[70]	+	-	-	-	+	+	+	-	-	Phrased	LCA-based
[326]	+	-	-	-	+	+	-	-	+	Mathematical	None
[103]	+	-	-	+	+	+	+	+	+	Phrased	Literature review
[327]	-	-	-	-	+	+	+	+	-	Partly	Literature review
[328]	+	-	-	-	+	+	+	+	-	None	None
[100]	+	-	-	-	+	+	+	+	-	Partly	Stakeholder engagement
[280]	+	-	-	-	+	-	+	-	-	None	LCA-based
[329]	-	-	-	-	+	-	+	-	-	None	LCA-based
[330]	+	+	+	+	+	+	-	-	+	Partly	None
[331]	+	-	-	-	+	+	-	-	+	Mathematical	None
[50]	+	+	+	-	+	+	+	-	+	Mathematical	Literature revie
[332]	+	-	-	-	+	+	+	-	-	Partly	None
[78]	-	-	-	-	+	+	+	-	+	Partly	None
[47]	-	-	-	+	+	+	+	+	+	Mathematical	None
[333]	-	-	-	+	-	-	+	+	-	None	LCA-based
[334]	-	-	-	+	-	+	+	-	+	Partly	None
[335]	-	-	-	-	+	+	+	+	-	Mathematical	None
[336]	-	-	-	+	-	+	+	-	-	Mathematical	None
[75]	+	+	+	+	+	+	+	-	+	Partly	None

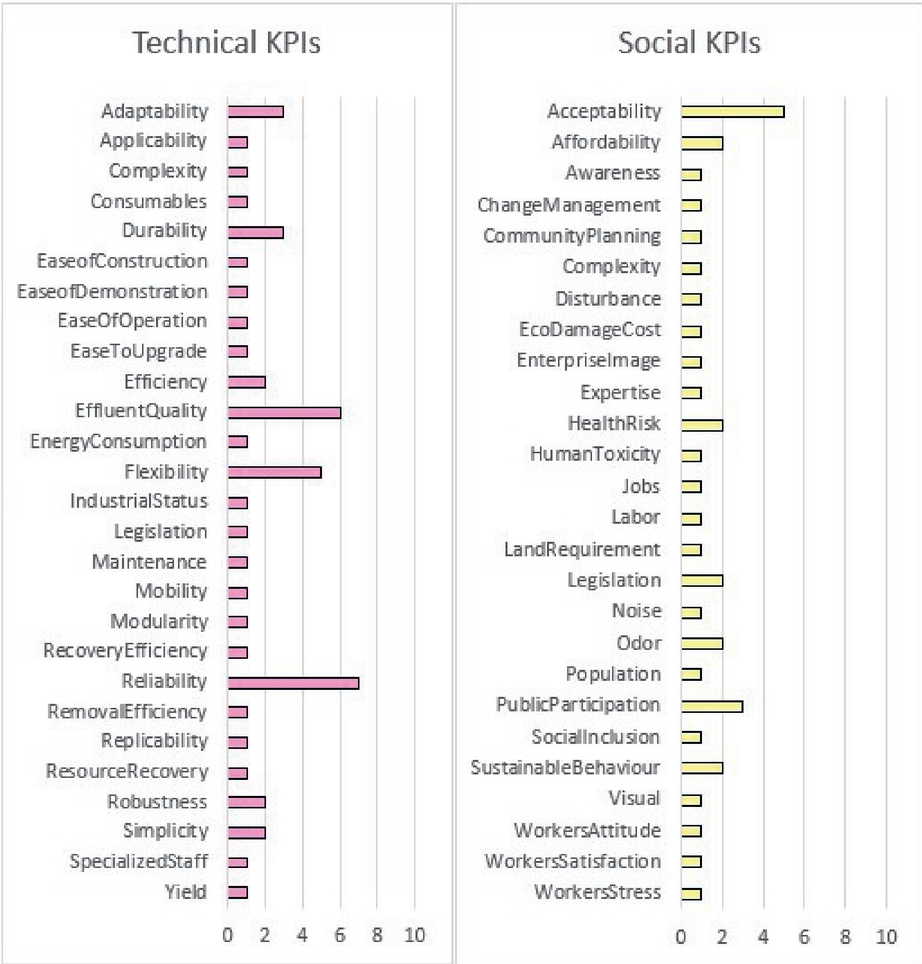

Figure A.1: *The number of the studies mentioning each technical and social indicator in the reviewed literature listed in Table A.1.*

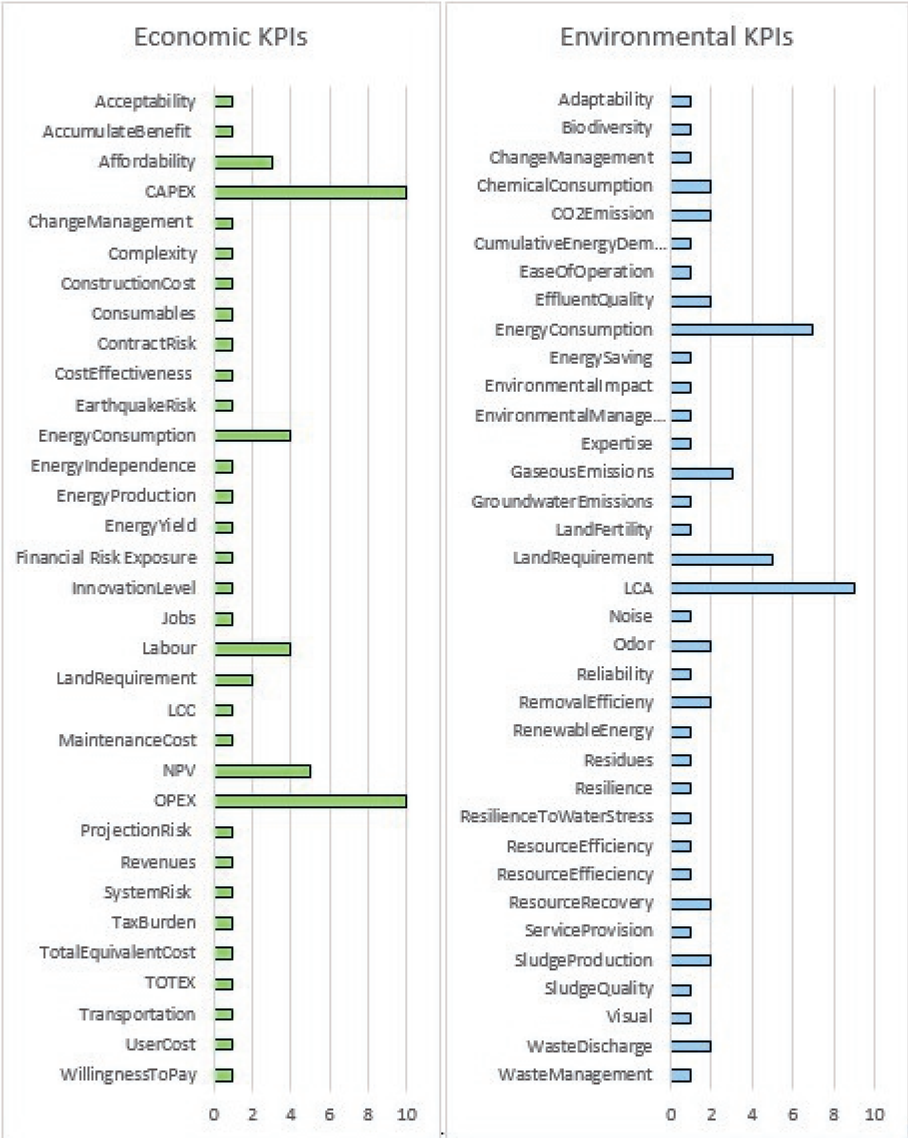

Figure A.2: *The number of the studies mentioning each economic and environmental indicator in the reviewed literature listed in Table A.1.*

A.3 Validation with partners

Table A.2: *The availability of characteristics for the unit processes (UPs) tested by the pilot partners. + means that data per characteristic is available; +/- means that data per characteristic is not available for all UPs in the TT; - means that data per characteristic is not available for any of the UPs in the TT.*

Characteristic per UP		**Unit**	**PP 1**	**PP 2**	**PP 3**	**PP 4**	**PP 5**
General	Type of the process	Scale 1 to 4	+	+	+	+	+
	Scale/Capacity	m3	+	+	+	+	+
	Area	m2	+	+	+	+	+
	Hydraulic retention time (HRT)	hours	+	+	+	+	+
	Level of noise emitted	dB	+/-	+/-	+/-	+/-	+/-
	Life time	years	+	+	+	+	+
	Component life time	years	+	+	+	+	+
Capital expenditure (investment costs)		euros	+	+	+	+	+
Operational and maintenance expenditures		euros/year	+	+	+	+	+
Min-max range	Temperature	°C	+/-	+/-	+/-	+/-	+/-
	pH	-	+/-	+/-	+/-	+/-	+/-
	Flow	m3/h	+/-	+/-	+/-	+/-	+/-
	Total suspended solids (TSS)	mg/L	+/-	+/-	+/-	+/-	+/-
	Chemical oxygen demand (COD)	mg/L	+/-	+/-	+/-	+/-	+/-
	Total nitrogen (TN)	mg/L	+/-	+/-	+/-	+/-	+/-
	Total phosphorous (TP)	mg/L	+/-	+/-	+/-	+/-	+/-
Recovery/removal	Water	%	+	+	+	+	-
	Total suspended solids (TSS)	%	+	+	+	+	+
	Chemical oxygen demand (COD)	%	+	+	+	+	+
	Total nitrogen (TN)	%	+	+	+	+	+
	Total phosphorous (TP)	%	+	+	+	+	+
	Heavy metals (Pb)	%	-	-	-	-	-
Log reduction	Virus, Bacteria	Log or %	+	+	+	+	+
Operation	Failure rate	%	+	+	+	+	+
Influent	Water flowrate	m3/h	+	+	+	+	+
	Total suspended solids (TSS)	mg/L	+	+	+	-	+
	Chemical oxygen demand (COD)	mg/L	+	+	+	-	+
	Total nitrogen (TN)	mg/L	+	+	+	+	+
	Total phosphorous (TP)	mg/L	+	+	+	+	+
	Heavy metals (Pb)	mg/L	+	-	+	+	-
	Bacteria (E. coli)	org/ml	-	-	-	-	-
Plant life time		years	+	+	+	+	+
Population size served		-	+	+	+	+	+

Table A.3: *The availability of context and resource-related characteristic and regulation. + means that data per characteristic or regulation is available for all cases; +/- means that data per characteristic or regulation is not available for all cases.*

Characteristics per country	**Abbreviation**	**Unit**	**Availability**
Net average income	NAI	euros/year	+
Climate change awareness	CCA	%	+
Climate change a threat	CC	%	+
Demand supply (DS) ratio per recovered resources	DS water	-	+
	DS N	-	+
	DS P	-	+
	DS energy	-	+
Characteristics per resources recovered			
Degree of human contact	HC water	%	+
	HC N	%	+
	HC P	%	+
	HC energy	%	+
Regulation / directive / etc.			
Limit concentrations (LC) effluent for discharge into the nature	LC TSS	mg/L	+
	LC COD	mg/L	+
	LC TN	mg/L	+
	LC TP	mg/L	+
Limit concentrations (LC) of heavy metal (HM)in the recovered resources	LC HM water	mg/L	+/-
	LC HM N	mg/L	+/-
	LC HM P	mg/L	+/-
E.coli concentration equivalent to 10^(-6) DALYS pppy	Cpe E.coli water	org/L	+/-
	Cpe E. coli N	org/L or org/kg	+/-
	Cpe E. coli P	org/L or org/kg	+/-

Appendix B. Supporting material for Chapter 4

B.1 Data for influent, location, resources

KPI parameters	KPI	Unit	RRP	WWTP	Notes and references	
Influent characteristics						
Q influent	PIG; OEP; FPT	m^3/hour	-	-	Varying per scale as explained in Chapter 4	-
IC TN	PIG	mg/L	-	-	Varying per scale as explained in Chapter 4	-
IC TP	PIG	mg/L	-	-	Varying per scale as explained in Chapter 4	-
IC COD	PIG; OEP	mg/L	-	-	Varying per scale as explained in Chapter 4	-
IC HM	ACC	mg/L	0,48	idem	((435888 kg Zn/year + 42237 kg Pb/year + 149586 kg Cu/year)*1000)/(Q influent *24 hours *365 days)/100 (100 treatment plants)	[337]
IC E. coli	ACC	cfu/100 mL	14000000	idem	1.4*10^8 cfu/L total E coli= 1.4*10^7 cfu/100 mL	[338]
Location and scenario characteristics						
HTT	PIG	hours	24	idem	-	-
DTT	PIG	days	365	idem	-	-
Required labour	OPEX; PIG	days/year	110	idem	-	-
	OPEX; PIG	months/year	12	idem	-	-
	OPEX; PIG	hours/day	8	idem	-	-
Salary	OPEX; PIG	€/h	37,5	idem	Estimated hourly labour costs, 2020	[339]
CCA	WTP	%	67%	idem	80% in 2017; 67% in 2019.	[340]
CCT	WTP	%	69%	idem	politician based 81% left wing, 55 % right-wing (47% of EU citizens)	[341]
NAI	WTP; AFF	€/pppy	27.864	idem	For 2020 montly salary (incl. vakation money) * 12 months	[342]
PE	WTP; AFF	people	144.241	idem	Calculated PE: 144241=(1506m3/h*517,2mg/L*24h/d)/(54 g/BOD/p/d*2,4-to convert to COD); 115315 Population served by RWZI Walcheren;	[216]
r	WTP	%	6	idem	Economic Optimisation	[343]
LC HM, effluent	ACC	mg/L	-	1,3	Irrigation water: based on the BTO Rapport anf efgf: Limit copper (Cu): 0,2 mg/L; Limit zinc(Zn): 0,196 mg/L; Limit lead (Pb): 0,05 mg/L; Effluent for discharge: limit established only for lead (Pb) max 1,3 mg/l for any opensurface waterbody	[344, 345, 346]
LC E.coli, effluent	ACC	cfu/100 ml	-	500	Irrigation water (all purpose): based on the BTO Rappport and efgf for agriculture; Effluent for discharge (bathing water): 500 cfu/100ml for good quality.	[344, 345]

continued on the next page

KPI parameters	**KPI**	**Unit**	**RRP**	**WWTP**	**Notes and references**	
Resource characteristics						
DS water	ACC		33,40%	idem	Average of ratio 20-40% for The Netherlands	[347]
DS TN	ACC		39,93%	idem		[348]
DS TP	ACC		481%	idem	Western Europe: suply capacity: 482 thousand tonnes; Total demand: 601+1718 thousand tonnes in 2018	[348]
DS Energy	ACC		103%	idem	Consumption 120 billion kWh, supply 117 billion kWh in 2017	[349]
Energy price	PIG	€/kWh	0,1376	idem	Industrial price for electricity in 2020: 0,1376 eurs/kWh; household price for electricity in 2020: 0,1427 eurs/kWh	[350]
VRP TN	PIG	€/kg	2	-	But can vary a lot depending on the quality	[351]
VRP TP	PIG	€/kg	1,7	-		[55]
VRP Biogas	PIG	€/Nm^3	0,688	-	caloric value of enriched and filtered biomethane: 7781.6 kJ/Nm3 and its energy generation capacity is 5 kWh/Nm3; industrial price for electricity in 2020: 0,1376 eurs/kWh; household price for electricity in 2020: 0,1427 eurs/kWh (This is only needed for some scenarios); so VRP energy=5*0,1376	[352, 350, 353, 353]
VRP Water	PIG	€/m^3	0,06	-	But can vary a lot depending on the availability; needs: 200 m^3/ha; In Zeeland, farmers pay 59.71 €/ha annually to the Water Board Scheldestromen	[354, 355]
LC HM,water	ACC	mg/L	0,446	-	Irrigation water: based on the BTO Rappport anf efgf: Limit copper (Cu): 0,2 mg/L; Limit zinc(Zn): 0,196 mg/L; Limit lead (Pb): 0,05 mg/L; Effluent for discharge: limit established only for lead (Pb) max 1,3 mg/l for any open surface waterbody	[345, 344, 346]
LC HM,TN	ACC	mg/kg N	9500	-	In fertilisers: max mgCu/kg N 1500; max mgZn/kg N 6000; max mgPb/kg N 2000	[356]
LC HM,TP	ACC	mg/kg P	11875	-	In fertilisers: max mgCu/kg PO4 1875; max mgZn/kg PO4 7500; max mgPb/kgPO4 2500	[356]
Cpe E. coli,water	ACC	cfu/100 ml	2,2	500	Irrigation water (all purpose): based on the BTO Rappport and efgf for agriculture; Effluent for discharge (bathing water): 500 cfu/100ml for good quality	[357, 345]
Cpe E. coli,TN	ACC	cfu/100 ml	100000	-	No limit in Dutch regulation but based on the offical journal of the European Union	[345, 356]
Cpe E. coli,TP	ACC	cfu/100 ml or cfu/100g	100000	-	No limit in Dutch regulation but based on the offical journal of the European Union	[345, 356]
HC irrigarion water	ACC	-	3	-	From van schaik et al 2021	
HC bathing water	ACC	-		4	Based on info in Chapter 2	-
HC TN	ACC	-	2	-	From Chapter 2	-
HC TP	ACC	-	2	-	From Chapter 2	-
HC energy	ACC	-	1	-	From Chapter 2 2021	-

B.2 Data used per unit process

KPI par.	Unit	Unit porcess										
		DS	EC	AD	SP	NF	RO	AC	BS	SwC	ASwD	EBPR
HRT	h	0,10	4,00	8,00	3,00	1,00	1,00	4,00	0,10	1,00	8,00	0,00
A	m^2/m^3	0,01	0,00	0,04	0,07	0,01	0,01	0,32	0,01	0,02	0,33	0,03
OP	-	1	2	4	2	1	1	3	1	2	3	0
LNP_j	dB	65	30	25	45	55	55	25	65	25	25	25
Fr_j	-	0,01	0,25	0,05	0,05	0,05	0,10	0,05	0,01	0,05	0,05	0,10
TRL	-	9	4	9	9	6	9	2	10	9	10	9
Lifetime	years	10	15	20	30	5	5	20	15	30	25	30
Max. TSS	mg/L	8,E+03	1,E+03	3,E+04	1,E+03	5,E+01	1,E+01	5,E+01	1,E+09	1,E+03	8,E+02	8,E+02
Max. COD	mg/L	1,E+09	1,E+09	1,E+06	1,E+09	4,E+01	1,E+01	1,E+09	1,E+09	1,E+09	5,E+03	5,E+03
Max. TN	mg/L	1,E+09	1,E+09	1,E+09	5,E+02	4,E+01	5,E+00	1,E+09	1,E+09	1,E+09	1,E+09	1,E+03
Max. TP	mg/L	1,E+09	1,E+09	1,E+09	5,E+02	4,E+01	5,E+00	1,E+09	1,E+09	1,E+09	1,E+09	1,E+02
Min. TSS	mg/L	2,E+02	1,E+02	0,E+00	0,E+00	1,E+00	1,E-01	0,E+00	2,E+02	2,E+02	1,E+02	0,E+00
Min. COD	mg/L	0,E+00	0,E+00	1,E+03	0,E+00	5,E+00	5,E-01	0,E+00	0,E+00	0,E+00	1,E+02	1,E+02
Min. TN	mg/L	0,E+00	0,E+00	0,E+00	1,E+02	0,E+00	0,E+00	5,E+01	0,E+00	0,E+00	5,E+00	2,E+01
Min. TP	mg/L	0,E+00	0,E+00	0,E+00	1,E+02	0,E+00	0,E+00	1,E+01	0,E+00	0,E+00	1,E+00	5,E+00
TSS Rem.	%	80%	85%	30%	0%	100%	90%	70%	2%	70%	97%	0%
COD Rem.	%	10%	50%	75%	0%	75%	70%	123%	1%	50%	90%	90%
TP Rem.	%	0%	95%	0%	80%	90%	90%	62%	0%	50%	28%	95%
TN Rem.	%	10%	10%	0%	20%	40%	70%	45%	0%	15%	87%	0%
HM Rem.	%	10%	80%	80%	58%	90%	98%	60%	1%	30%	59%	0%

continued on the next page

KPI par.	**Unit**	**Unit porcess**										
		DS	**EC**	**AD**	**SP**	**NF**	**RO**	**AC**	**BS**	**SwC**	**ASwD**	**EBPR**
Log Bac. Rem. *	log	0	1,70	4	1	4	5,50	1	0	1,70	1,70	0
Log Bac. Rem. **	log	-	0,01	-	0,05	-	0	0,05	-	0,01	0,01	-
Bac. Rem.	%	0%	98%	100%	90%	100%	100%	90%	0%	98%	98%	0%
Water Rem.	%	0%	10%	1%	1%	17%	25%	30%	0%	10%	10%	0%
COD Rec.	%	-	-	45%	-	-	-	-	-	-	-	-
Water Rec.	%	100%	90%	99%	99%	83%	75%	70%	100%	90%	90%	100%
Capex B	-	0,51	0,20	0,52	1,00	0,84	0,84	0,59	0,51	0,47	0,72	0,52
Capex C	-	4,04	29,83	1,70	0,18	1,01	1,01	3,10	4,04	29,05	8,22	1,70
Land B	-	0,52	0,00	0,96	1,00	0,50	0,50	0,29	0,52	1,02	1,00	0,96
Land C	-	0,00	0,00	0,00	0,00	0,00	0,00	0,02	0,00	0,00	0,00	0,00
Energy B	-	1,01	1,10	1,00	0,95	1,00	1,00	1,00	0,00	1,00	1,00	1,00
Energy C	-	4,14	5,30	1,82	147,73	164,28	365,00	27,40	0,00	1,30	183,32	1,82
Labour B	-	0,00	0,00	0,00	0,24	0,18	0,18	0,06	0,00	0,05	0,14	0,00
Labour C	-	4,00	24,00	0,00	17,41	57,02	57,02	51,15	4,00	12,85	159,86	0,00
Opex B	-	0,49	0,50	0,59	1,10	1,35	1,10	0,01	0,49	0,52	0,92	0,59
Opex C	-	0,46	0,74	0,05	0,01	0,00	0,01	13,03	0,46	1,56	0,08	0,05

*going to the side stream so account for the main stream
**going to the main stream so account for the side stream
The B's and C's are coefficients as proposed by [75]

C.1 Calculation methods

C.1.1 Temperature correction

The methods applied int his study to correct flux and solute retention for temperature are provided in Equation C.1 and Equation C.1.2, respectively.

$$J_{W25} = J_{Wt} * \frac{\mu_{25}}{\mu_t} \tag{C.1.1}$$

$$SR_{25} = SR_t * \frac{\mu_t}{\mu_{25}} \tag{C.1.2}$$

where J_{W25} and SR_{25} are the permeate flux and the solute rejection at 25°C, J_{Wt} and SR_t are the permeate flux and the solute rejection at the experimental temperatures, μ_t and μ_{25} are the water viscosity at the experimental temperatures and at 25°C, respectively.

C.1.2 Normalisation

In this study, first the normalised B values were estimated with normalised fluxes using Equation C.1.3 and Equation C.1.4). Then the normalised B values were re scaled as presented in Equation C.1.5.

$$B_{norm} = \frac{J_{norm}}{SR_{25}} * (1 - SR_{25}) \tag{C.1.3}$$

$$J_{norm} = \frac{J_{w25}}{J_{max25}} \tag{C.1.4}$$

$$B = J_{max25} * B_{norm} \tag{C.1.5}$$

where B_{norm} is the normalised B value, J_{norm} is the normalised fluxes (J_{w25}) using the maximum flux from the dataset (J_{max25}), and SR_{25} is the solute rejection, all corrected for temperature.

C.1.3 Energy and area requirement

Pumping power (q, kW) which can be quantified as presented in Equation C.1.6 (Nilsson et al. 2008; Villain-Gambier et al. 2020).

$$q = \frac{Q * TMP}{\eta_{pump}} \tag{C.1.6}$$

where q is the pumping power in kW, Q is the flow rate m^3/s, TMP is the trans-membrane pressure in Pa, since this study assumes a single stage NF, and η_{pump} is the pump efficiency in %, in this study assuming it to be 70% so η_{pump}=0.70. The membrane area requirement was quantified as shown in Equation C.1.7.

$$Area = \frac{Q * R_w}{J_w} * F \tag{C.1.7}$$

where $Area$ is the total required membrane area in m^2, Q is the influent flowrate in L/h, R_w is the targeted water recovery in %, J is the permeate flux in $L/m^2.h$ and F is a factor representing the assumption that the actual area actually required is larger than the theoretical value, in this study assuming it to be 15% so F=1.15.

C.2 Optimisation model output for scenarios with specific targets

Five scenarios with specific targets for water recovery and component rejections were used to discuss the sensitivity of the optimisation model. The optimisation model outputs are presented in Table C.2.1.

Changing the targets did have an influence on both the selected membrane and the TMP and therefore on the energy and surface area requirements. Reducing the water recovery target from 70% (BC) to 50% (BC-W50) or increasing it to 90% (BC-W90), while keeping the water quality targets the same, resulted in the selection of the same membrane and TMP as the base case: NF270 and 8 bar. Therefore, the only difference between these three scenarios was the surface area requirement: BC-W50, recovering 20% less water required 29% less surface area and BC-W90, recovering 20% more water required 29% more surface area.

If the target water recovery is 90% but no water quality targets are set (M-W) the optimisation model chose the NF90 membrane and a TMP of 12 bar. This can be explained by the fact that in the absence of permeate quality targets the model optimises between maximising recovered water quality, while minimising associated energy and area requirement. This way the permeate quality improved in terms of COD and TN in comparison with the base case, with 16% and 58% higher removals, respectively. The removal of TP however decreased from 92% (BC) to 88% (M-W). The associated area and energy requirement for the selected membrane and TMP increased with 56% and 50% respectively, in comparison with the base case (BC). This is in accordance with the differences in the area and energy costs for the two membranes at various TMPs.

Maximising the removal of all components while keeping the water recovery the same as in the base case (BC-M-RCNP), resulted in the selection of membrane NF90 and a TMP of 21 bar. The NF90 was chosen as this membrane has a smaller MWCO and is better in removing components, especially TN. The chosen TMP was the highest of all these scenarios, mostly to ensure high removal of TN. The selected TMP resulted in the highest energy requirements and thus energy costs, yet the lowest required area of all these scenarios.

Setting no target for COD removal, while maximising the removal of TP and the permeation of TN and keeping the water recovery the same as the base case (BC-M-RP-PN) resulted in the selection of the membrane NF270, the same as for the base case (BC). The selected TMP was 6 bar, 2 bar lower than the for the base case (BC), mostly to favour permeation of TN: 8.20 mg/L TN, just 0.14 mg/L more than base case. The lower selected TMP for this scenario resulted in the

Table C.2.1: *Optimisation model output for the scenarios* with different targets for permeate in terms of: quantity (% recovery) and quality (concentration of COD, TN, and TP in mg/L). Colour coding: blue-water recovery percentage and flux, yellow-achieved solute rejection (SR), red-area and associated costs, green-energy and associated costs.*

Scenarios			Unit	BC	BC-W50	BC-W90	M-W	BC-M-RCNP	BC-M-RP-PN
Model input	Influent	Base case				Base case			
	Targets for the permeate	Water	%	70	50	90	90	70	70
		COD	mg/L	≤ 12	≤ 12	≤ 12	-	≤ 4	-
		TN	mg/L	≥ 4	≥ 4	≥ 4	-	≤ 0,9	≥ 6
		TP	mg/L	≤ 0,1	≤ 0,1	≤ 0,1	-	≤ 0,05	≤ 0,05
Model output	Selected	Membrane		NF270	NF270	NF270	NF90	NF90	NF270
		TMP	bar	8	8	8	12	21	6
	Permeate quality	Flux	$L/m^2.h$	87,1	87,1	87,1	63,8	111,6	58,1
		COD	mg/L	11,68	11,68	11,68	5,25	3,18	14,2
		TN	mg/L	8,06	8,08	8,08	3,11	2,1	8,2
		TP	mg/L	0,04	0,04	0,04	0,06	0,04	0,05
	Achieved solute rejection (SR)	COD	%	71	71	71	87	92	65
		TN	%	6	6	6	64	75	4
		TP	%	92	92	92	88	93	90
	CAPEX and OPEX	Area	m^2	15654	11181	20126	24427	10856	20872
		A cost	€/m^3	0,18	0,13	0,23	0,28	0,13	0,24
		q	kW	478	478	478	717	1255	358
		E cost	€/m^3	0,3	0,3	0,3	0,45	0,78	0,22

*BC: base case permeate quality and quantity (70% water recovery); BC-W50: base case permeate quality but 50% water recovery; BC-W90: base case permeate quality but 90% water recovery; M-W: maximize water recovery with flexible permeate quality; BC-M-RCNP: base case permeate quantity but maximize rejection of COD, TN, and TP; BC-M-RP-PN: base case permeate quantity but flexible COD rejection, maximize TP rejection, and maximize TN permeation.

least energy of all five and thus a lower OPEX, which was 0.08 €/m^3 lower than the base case (BC). On the other hand, the required area was one of the highest of all five scenarios, 0.06 €/m3 more than the base case. This can be explained by the low TMP resulting in the lowest flux, about 29 $L/m^2.h$ lower than the base case while the water recovery target was the same as for the base case (70%).

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SUMMARY

Urban wastewater has been proven to contain valuable resources. Starting from the organic matter, the nutrients, and the water itself, various products can be extracted, processed, and reused safely. Many different technologies for recovery of resources have been developed, tested, and applied for decades already. The variety of processes but also of recoverable products has been growing exponentially. At the same time, requirements are imposed on wastewater treatment and resource recovery plants to become more efficient, cost-effective, and environmentally friendly. For all these reasons, it has been increasingly difficult for decision-makers to choose the most feasible option for wastewater treatment and resource recovery in their specific situation.

Choosing the most feasible option for resource recovery from urban wastewater implies selecting a number of compatible unit processes that can form a treatment train capable of treating a given wastewater stream and simultaneously recovering the targeted resources. The most feasible treatment train would be the optimal option in terms of technical, economic, environmental, and social criteria. Model-based evaluation and design frameworks and tools have been demonstrated to be able to deal with such multi-dimensional problems. Nevertheless, as concluded in **Chapter 1**, there is a lack of such frameworks and tools and consequently a lack of clarity about what information is needed and how it can be used best in digital tools for decision-making by wastewater managing organisations and supporting advisors.

Therefore, this thesis aimed at exploring the building blocks of decision-making for resource recovery from urban wastewater. For this, the three main objectives were:

- Identify what information is needed to (i) perform a model-based evaluation of impacts and (ii) design resource recovery treatment trains;
- Develop models for treatment train design, evaluation, and optimisation;
- Explore ways to improve the models for treatment train design.

The resources accounted for in this thesis were water (i.e. drinking water and irrigation water), energy (i.e. chemical energy represented by COD), and nutrients (i.e. nitrogen represented by TN and phosphorus represented by TP). Chapter 1 also motivates the focus on these resources and presents the most commonly used processes for recovering these resources as well as the current practices for decision-making.

For model-based impact evaluation and design of treatment trains, a set of key performance indicators (KPIs) were defined and mathematically formulated in **Chapter 2**.The selected set of KPIs (i.e. two technical, four economic, four environmental, and four

social) was shortlisted from literature by the NEREUS Interreg 2 Seas project stakeholders. Existing mathematical formulations and phrased definitions were searched for in the literature. When a KPI had already been mathematically formulated, its applicability for resource recovery from urban wastewater was checked and when needed further tailored for practical use. For design purposes, the KPIs had to incorporate characteristics of unit processes, the local context, and the resources to be recovered. Some of the environmental and social KPIs represented constraints ensuring the viability of treatment trains. The applicability of the proposed KPIs was checked with the NEREUS pilot partners, indicating which KPI is quantifiable with the current process monitoring programmes. In this way, this chapter highlighted the importance of aligning information from technology suppliers with the required information for decision-making.

Most of the KPIs which were defined and mathematically formulated in Chapter 2, were used to build the conceptual framework for decision-making presented in **Chapter 3**. This framework was developed such that for a wastewater treatment plant influent and targeted resources a number of compatible treatment and recovery processes is automatically selected from a unit process library. The main building blocks of the conceptual framework were: user input, knowledge library, optimisation model, and model output. The requirements of the user input and the knowledge library are very much determined by the parameters incorporated in the mathematical formulation of each KPI. The user input requires influent quality and quantity specifications as well as the target resources, the country, and weighting per indicator and criterion. The knowledge library contains information about the unit process, the recoverable resources, and the country in which the treatment trains would be placed. With this information, the optimisation model (i.e. weighted multi-objective multi-integer non-linear programming, WMOMINLP) generates the model output consisting of the treatment train, the KPI values, the approximate amount of recovered resources, and the effluent quality in case water recovery is not targeted. The model selects compatible unit processes based on: (i) the COD concentrations in the influent and the minimum and maximum allowed COD per unit process, (ii) the task that a unit process can perform (i.e. energy recovery, phosphorous recovery, nitrogen recovery, water disinfection) and (iii) whether the unit process can perform the task in the main or a side stream. However, it does not provide the position of the unit processes in the treatment train. This requires additional heuristics with logical ('if-then') rules from experts which could be explored in future research.

Some of the KPIs from Chapter 2 were also used in **Chapter 4** to compare conventional and new configurations for wastewater treatment and resource recovery. The method applied in this chapter was a multi-criteria decision analysis. A normalisation method applied to the KPIs values and weighting applied to both KPIs and criteria enabled the scoring and ranking of the scenarios. A sensitivity analysis of the influent quality and quantity, plant size, and criteria weighting was carried out to evaluate the effect of these on the scores and ranking of scenarios. With equal weighting of KPIs and criteria, the new configurations scored better than the conventional ones for the environmental criteria but worse for the technical and economic criteria. From a social perspective, the scores of the new and conventional configurations were similar. In the sensitivity analysis, only plant size and criteria weights affected the ranking of scenarios within both ranking per criterion and overall ranking. At large plant sizes, the conventional configurations scored better than the new ones, while at medium and small plant sizes the new configurations scored better. The results of this study demonstrated the importance of accounting for weighting and scale in decision-making upon resource recovery from urban wastewater.

As a possible improvement for the framework presented in Chapter 3, **Chapter 5** explored the potential of a grey-box modelling approach for nanofiltration to include process performance ranges rather than fixed performance efficiency numbers. For this, the water flux and solute (i.e. COD, TN, and TP) retention efficiency were modelled as a function of transmembrane pressure (TMP) for two nanofiltration membranes with different pore size (i.e. molecular weight cut-off, MWCO). The applicability of the model was demonstrated through an optimisation model finding the optimal membrane and TMP by minimising capital and operational costs. A sensitivity analysis of the influent and the targeted resource recovery (i.e. water, COD, TN, and TP) was carried out to evaluate the robustness of the optimisation. The results showed no sensitivity to influent characteristics but when changing the targets for recovered water quality and quantity, the optimisation model selected different membranes and TMPs. Thus, this study demonstrated that it is important to account for process configuration and operational details in decision-making. The sensitivity of a full treatment train design (Chapter 3) to varying process performance still needs to be tested in future research.

The contribution and limitations of the results of this thesis are discussed in **Chapter 6**. and summarised with the following topics: quantitative evaluation of qualitative aspects, feasibility goes beyond compatibility, pollution control and resource recovery, process modelling for improved decision making, and supporting the transition from wastewater treatment to resource recovery. Furthermore, the novelty of the work presented in this thesis was discussed in comparison to a few simultaneous developments in the field, which either focus on the recovery of only one resource or solely on the recovery of resources without considering wastewater treatment or do not provide the model for treatment train design. Nevertheless, these have elements worth considering for future developments of the framework presented in this thesis such as other resources, the reuse of resources, more regional aspects, and generating more than one treatment train as an output for model-based design. Finally, this chapter ends with an overview of recommendations for future research and developments including extending the system boundaries for model-based evaluation and design through extensive comparative research for process modelling (i.e. black- vs. grey- vs. white-box modelling) and exploring ways to integrate tools like Life cycle Analysis (LCA) for more global impact evaluations and Geographical Information System (GIS) for local and regional resource reuse planning.

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