1 Towards the Synthesis of Wastewater Recovery Facilities using Enviroeconomic Optimization

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The wastewater treatment industry is undergoing a major shift towards a proactive interest in recovering materials and energy from wastewater streams, driven by both economic incentives and environmental sustainability. With the array of available treatment technologies and recovery options growing steadily, systematic approaches to determining the inherent trade-off between multiple economic and environmental objectives become necessary, namely enviroeconomic optimization. The main objective of this chapter is to present one such methodology based on superstructure modeling and multi-objective optimization, where the main environmental impacts are quantified using life cycle assessment (LCA). This methodology is illustrated with the case study of a municipal wastewater treatment facility. The results show that accounting for LCA considerations early on in the synthesis problem may lead to dramatic changes in the optimal process configuration, thereby supporting LCA integration into decision-making tools for wastewater treatment alongside economical selection criteria.

1.1 INTRODUCTION

Untreated sewage presents a threat to human health and the environment. For the most part, wastewater treatment design retains its foundations in engineering traditions established in the early 20th century [17]. The aerobic treatment processes used to produce an effluent that complies with the discharge standards are often energy intensive, and may be significant contributors to greenhouse gas (GHG) emissions including carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O) [14]. Moreover, large quantities of sludge may be produced as a by-product of aerobic treatment, and wastewater treatment facilities can also be land demanding. However, a paradigm shift is underway towards making wastewater treatment facilities more sustainable, driven by a range of sustainability issues including increase in electricity demand and price [34], and long-term nutrient scarcity and high extraction costs [7, 53]. In this new paradigm, wastewater is regarded as a renewable resource from which water, materials and energy can be recovered, thereby transitioning to resource recovery facilities [29].

Because wastewater treatment is often regarded as being an end-of-pipe technology, the design of wastewater treatment facilities tends to focus on minimizing the environmental impacts of given contaminants present in the effluent, such as organic matter (COD), nitrogen (N) and phosphorus (P). Indeed, many environmental regulations still focus on the removal of these targeted contaminants without consideration of the broader environmental issues. Nowadays there is a greater awareness that sustainability objectives, beyond receiving water quality, should be accounted for in the design and operation of wastewater treatment facilities, in response to which there has been much research emphasis on life cycle assessment (LCA) in the wastewater treatment industry in recent years.

LCA is a holistic, cradle-to-grave standardized approach to evaluating the environmental impacts of products and services [35]. As far as wastewater treatment is concerned, LCA was first applied in the 1990s for identifying the environmental impacts of various small-scale wastewater treatment technologies [21]. Since then, it has been increasingly used in this industry as a means of comparing different wastewater treatment technologies [27, 25, 67] or sludge management technologies [72], and for evaluating the main environmental impacts associated with specific wastewater treatment processes [73, 58]. The sensitivity of the LCA results to various impact assessment methods has also been investigated [64]. As pointed out in a recent review paper [16], however, there is a need for better linking LCA with economic and societal assessments in order to provide a more complete and accurate sustainability picture for decision makers.

An approach to incorporating LCA evaluation into a knowledge-based decision-support system to design wastewater treatment plants (WWTPs) has recently been presented in [28]. The results demonstrate the potential of LCA for decision making, although the approach is largely dependent on the data quality and their specifications [37]. Moreover, this approach may not provide further information with regards to the optimal (or near-optimal) solutions. In essence, superstructure optimization [10] provides an ideal framework to identify optimal solutions of those design problems having a large number of alternative processes, and it may be combined with multi-objective optimization in the presence of multiple conflicting objectives, e.g. economic and environmental performance indicators. This approach has been successful in various application areas, including the synthesis of water networks [2, 39, 61], as well as wastewater treatment and resource recovery systems [65, 60, 13]. Because it is computationally demanding, the key to its success is the development and selection of mathematical models for the units that are simple enough for the optimization problems to remain tractable, yet provide reliable estimates of their performances and associated costs.

The main objective of this chapter is to present a modeling methodology for decision in wastewater treatment and resource recovery systems in order to arrive at WWTP designs that are both environmentally sustainable and economically viable, namely enviroeconomic optimization. This methodology is based on superstructure modeling and multi-objective optimization, where the main environmental impacts are quantified using life cycle assessment (LCA). Moreover, these developments are illustrated with a simple case study in municipal wastewater treatment. The rest of this chapter is organized as follows: a review of resource recovery and WWTP design is first presented (Sect. 1.2), followed by the methodology (Sect. 1.3) and illustrative case study (Sect. 1.4), before drawing conclusions.

1.2 BACKGROUND

1.2.1 RESOURCE RECOVERY FROM WASTEWATER

This subsection reviews various technologies for recovery of energy and materials from wastewater, with an emphasis on proven technologies. For further details, we refer the reader to the recent survey/perspective articles [53, 7].

The organic compounds present in municipal (and many industrial) wastewaters can be converted into a methane-rich biogas via anaerobic digestion. It is estimated that about 30-60 L/d of methane per capita can be generated from a typical municipal wastewater by transforming all of the biodegradable organic matter into biogas [57]. Moreover, anaerobic digestion can be adopted in conjunction with downstream resource recovery units due to its minimal effect on ammonia or phosphate removal. In contrast to biogas generation from high-strength wastewater and wastewater sludge that has been employed for many years, direct anaerobic treatment of low-strength wastewater has not been widely practiced so far, especially in temperate climates where wastewater temperature is in the range of 5-15°C. Innovations in reactor design to maintain elevated biomass inventories, such as the upflow anaerobic sludge blanket (UASB) and anaerobic membrane bioreactor (AnMBR), have mitigated some of the limitations and have extended the range of applications of anaerobic treatment [46, 45, 52]. Particularly promising configurations include the submerged anaerobic membrane bioreactor (SAnMBR; [33, 48]) and, more recently, the anaerobic fluidized membrane bioreactor (AFMBR; [40]). Research is underway to develop improved membranes and reactor designs that reduce membrane fouling and enhance dissolved methane recovery [68, 70]. In urban water systems, thermal energy can be recovered through the use of heat pumps or heat exchangers. Although in the form of low-grade energy due to small temperature differences, this energy may be suitable for heating buildings [22]. Besides biogas and thermal energy, promising technologies for electricity or hydrogen generation from wastewater are also emerging [50, 41].

Nitrogen (N), phosphorus (P), and potassium (K) are critical nutrients for intensive agriculture, whereas there has been increasing concern about the long-term scarcity or high extraction cost associated with these nutrients; Phosphorus is a non-renewable mineral resource, which is fast depleting. It is estimated that the worldwide phosphorus demand will outstrip supply within a few decades as a consequence of an expanding population, which has major implications in terms of global food security as 90% of the phosphate (PO_4^{3-}) rock reserves are located in just five countries [53]. There has been little discussion regarding potassium as a macro-nutrient target for recovery so far, although its price is projected to rise substantially in the next decade due to a limited geological distribution [7]. Fertilizer production is also highly reliant on the energy-intensive and natural gas-dependent ammonia production process. The rising natural gas market price in past decades is projected to continue (doubling by 2025), which will directly affect the price and supply of nitrogen fertilizers [7]. In this context, much research has been dedicated to N and P recovery from nutrient-rich wastewater in recent years [20, 44, 69]. In the presence of a precipitating or fixing agent, a majority of the phosphates – which accounts for 50-80% of the total P compounds in municipal wastewater [75] – can be recovered. Moreover, technologies for recovering soluble N compounds from municipal wastewater – around 50-80% of the total N content [75] – are becoming economically viable. Ion exchange, for instance, can recover either ammonia, nitrate or phosphates by passing the secondary effluent through adsorbent columns and chemical regeneration [47, 36], and the resulting nutrient-enriched solutions can be further processed into a saleable product (e.g., fertilizer). Nonetheless, key challenges for the wider deployment of ion exchange units include their potential for fouling with suspended solids, the limited exchange capacity of certain adsorbents, the limited ion selectivity, and their high capital costs [54]. A range of absorbents are available, which include zeolites (e.g. clinoptilolite) for ammonium ions (NH_4^+) fixation [3, 78] and polymeric resins with higher exchange capacities. Research is also underway to develop anion adsorbents with high phosphate selectively and easy regeneration characteristics, including hydrotalcite (HTAL) [43] and polymeric resins with hydrated ferric oxide nanoparticles [51]. An alternative promising technology for P recovery is reactive filtration, which combines physical filtration of particulate P compounds with co-precipitation and adsorption of soluble P compounds onto coated sand in a moving bed filter – up to 95% P recovery by using hydrous ferric oxide (HFO) coated sand [56]. In addition, adoption of crystallization for P recovery from concentrated wastewater streams has attracted substantial interest to produce reusable compounds such as calcium phosphate ($Ca_3(PO_4)_2$) and struvite ($MgNH_4PO_4$) [44]. The recovery technology involves precipitation in either stirred tanks or fluidized bed reactors [9], with the latter being the most commonly applied in struvite crystallization. Note, however, that most nutrient recovery technologies to date have been applied to sludge liquors with PO_4^{3-} concentrations of 50-100 mg/L, for which 80% removal efficiencies or higher have been reported [76]. For dilute streams, such as secondary effluents with PO_4^{3-} concentrations of 4-12 mg/L, struvite crystallization may be combined with adsorbent columns and fed with the enriched solutions from the adsorbent regeneration e.g. RIM-NUT process reported by [47]. Besides N and P recovery, organic carbon too can be recovered as polyhydroalkanoates (PHAs) [15], whereas heavy metals can be recovered via adsorption, membrane filtration, or chemical precipitation [26].

1.2.2 DESIGN OF WASTEWATER TREATMENT FACILITIES

The traditional rules and guidelines for design of wastewater treatment facilities – see, e.g., Metcalf & Eddy [75] – are being challenged nowadays by tighter economic and environmental constraints. Moreover, with the extra degrees of freedom offered by advanced treatment and separation technologies, the plant synthesis/design problem becomes much more complex, especially when it comes to selecting the most sustainable wastewater treatment facilities in a given regional context [66].

Mathematical modeling has been a powerful tool in assisting decision making in WWTP design since the 1990s. Not only have the computational capabilities and numerical solution technology improved dramatically, but the mathematical models too have become more predictive, now enabling plant-wide simulation routinely using a range of commercial simulators (GPS-X®, BioWin®, WEST®, etc). Conventional model-based WWTP design starts with the selection of a plant layout, and then focuses on the detailed design and analysis of this particular layout. The selection of an appropriate design that meets the specified objectives and constraints involves comparing the capital and operating costs of multiple plant configurations, thus requiring repetitive model simulations alongside comprehensive process knowledge. As the number of processes and configurations increases, this design approach becomes more tedious, and ultimately unmanageable.

In order to deal with large numbers of treatment or separation units and possible interconnections, a system engineering approach is most useful. Systematic methods for the synthesis of complex chemical plants and biorefineries based on superstructure modeling and optimization are well developed [10, 42, 49]. These approaches are also increasingly applied to water network synthesis in process plants in order to minimize fresh water consumption and wastewater generation through regeneration, recycle and reuse [23, 39]. Regarding municipal wastewater facilities, the need for systematic approaches has been emphasized [6, 31], but relatively few studies have been published to date [65, 4, 5, 60, 13]. These studies provide insight into the potential of the systematic optimization-based approaches for wastewater treatment design, but they are nonetheless limited to optimizing a given process or selecting the most appropriate process among a small number of alternatives mainly based on economical considerations.

Another challenging task for WWTP design is satisfying multiple conflicting objectives simultaneously, while meeting the discharge regulations. One example is the trade-off between nutrient discharge targets and plant-wide energy consumption. Traditionally, these problems have been addressed using single objective optimization through weighting of the various contributions in an overall cost index. In contrast, multi-objective optimization provides a means of describing multiple objectives separately by determining the so-called Pareto solution set of non-dominated solutions [30]. This approach has not been applied widely in WWTP design to date, perhaps due to the complexity of wastewater treatment processes. A decision-making tool to support the design of WWTPs based on multi-criteria evaluation was proposed in [24], The selection of different process alternatives in this tool is based on an overall degree-of-satisfaction index, as obtained through the weighting of selected criteria and objectives, and it relies on a mix of mathematical modeling and qualitative knowledge. Another interactive multi-objective optimization platform coupled with model-based simulation, called NIMBUS, was presented in [30]. This platform allows a decision maker to simultaneously consider the design of WWTPs from different standpoints, and to balance between the different objectives. More recently, an integrated framework combining LCA with dynamic simulation to compare different treatment processes was developed in [12], with a focus on source separation and energy/nutrient recovery. On the whole, these existing approaches are certainly heading in the right direction, but the exploration remains limited to a small number of process configurations nonetheless. In contrast, the following sections present and illustrate a superstructure modeling and optimization methodology, which addresses some of these limitations.

1.3 METHODOLOGY

The combination of traditional wastewater treatment technology with advanced energy and materials recovery solutions offers considerable promise to improve the sustainability and reduce the cost of wastewater facilities. Clearly, the ultimate goal here is a closed cycle, energy-sufficient process, where all waste streams are recycled and the only output is saleable/valuable products. This section investigates the question as to how to select and interconnect, from a wide variety of unit operations, those units which will lead to the most sustainable wastewater treatment systems – a problem known as synthesis or flow-sheeting in process engineering.

The synthesis problem statement starts with the specification of the following data:

- A set of wastewater streams of given flow rates and compositions;
- A set of water sinks with known maximum concentration limits or financial penalties as defined by local/federal authorities;
- A set of treatment and separation units with given performance for targeted compounds and associated costs and environmental burdens.

These specifications can be represented by a generic superstructure, which considers every possible interconnection in a fixed network topology. One such superstructure is illustrated in Fig. 1.3, for a simple network topology that consists of a single wastewater stream, two sinks (treated effluent and biosolids), and a range of treatment/separation units. The objective of the synthesis problem is to determine an optimal resource recovery facility in terms of: (i) its units; (ii) the piping interconnections between the units; and (iii) the flowrates and compositions in the interconnections. Here, *optimal* is understood in terms of maximizing the net present value (NPV) and minimizing given environmental impacts.

1.3.1 SURROGATE-BASED OPTIMIZATION

Mathematically, superstructure optimization problems can be formulated as optimization models with two types of decisions:

- the discrete, usually binary, decisions on the units that should be included in the system along with their interconnections, here denoted by y; and,
- the continuous decisions that define the flows and compositions as well as certain design and operating parameters, here denoted by x.

This leads to multi-objective mixed-integer nonlinear programs (MO-MINLP) in the form:

$$\begin{aligned} \min_{x,y}\ & [\mathrm{KPI}_1(x,y), \mathrm{KPI}_2(x,y), \ldots] \\ \text{s.t.}\ & h(x) = 0 \\ & g(x,y) \leq 0 \\ & x \leq 0, y \in \{0,1\}\,. \end{aligned} \tag{P}$$

The objective of the MO-MINLP consists of minimizing two or more key performance indicators (KPIs), which are functions of both types of variables. These variables must also satisfy restrictions of the form $g(x,y) \leq 0$, either design specifications in terms of discharge allowance and physical operating limits, or logical constraints for the existence of piping interconnections with nonzero flows or the sequencing of certain units. Last, but not least, the continuous variables x must obey material balance equations of the form $h(x) = 0$, where usually $\dim(h) < \dim(x)$, describing models of the physical units.

A key element of the superstructure optimization approach is that these latter models should remain as simple as possible in order to comply with state-of-the-art algorithms and computational capabilities, thereby calling for a surrogate-based approach for the synthesis problem. Previous work by [60] advocates for the use of surrogate models constructed from state-of-the-art WWTP simulators as depicted in Fig. 1.1. In order to determine solutions that are accurate enough, the most promising process alternatives determined from the superstructure optimization problem (P) are then validated against the simulator-projected performances and costs. Typically, this would create an iteration between the superstructure optimization and the simulator for refining the surrogates. In particular, recent developments in surrogate-based optimization can provide guarantees that the iterations will converge to a (local) optimum with minimum recourse to high-fidelity models [1, 11]. Finally, the selected process candidates can be considered for detailed performance and cost analyses, including integration options and operability issues. To account for additional design and operational constraints, further iterations with the superstructure optimization block may then be necessary.

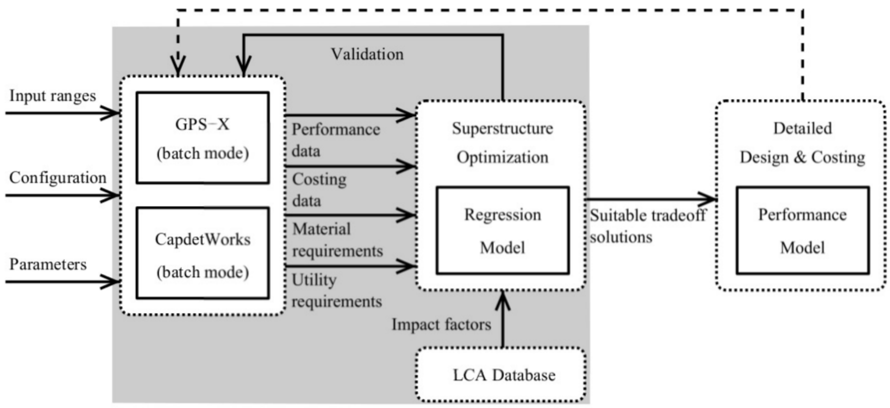

Figure 1.1 Illustration of the proposed methodology based on multi-objective superstructure optimization and surrogates models [77]

The following subsection presents an approach to deriving surrogate models for predicting plant-wide performance. Then, the computation of economic and environmental performance indicators is discussed in Sects. 1.3.3 and 1.3.4. Finally, numerical solution considerations are discussed in Sect. 1.3.5.

1.3.2 PLANT-WIDE PERFORMANCE SURROGATES

Performance models in the superstructure optimization problem (P) are based on the material balances on flows (F) and concentrations (X) around the sources, the units and the sinks. For instance, the material balances for a given species c in the treatment unit k can be formulated as [60]:

$$\begin{aligned}
F_k^{\text{in}} &= \sum_{i=1}^{N_{\text{source}}} F_{i\to k} + \sum_{k'=1}^{N_{\text{unit}}} F_{k'\to k}\\
X_{k,c}^{\text{in}} F_k^{\text{in}} &= \sum_{i=1}^{N_{\text{source}}} F_{i\to k} X_{i,c} + \sum_{k'=1}^{N_{\text{unit}}} F_{k'\to k} X_{k',c}^{\text{out}}\\
X_{k,c}^{\text{in}} F_k^{\text{in}} (1-\rho_{k,c}) &= \sum_{k'=1}^{N_{\text{unit}}} F_{k\to k'} X_{k,c}^{\text{out}} + \sum_{j=1}^{N_{\text{sink}}} F_{k\to j} X_{k,c}^{\text{out}}\,,
\end{aligned}$$

where the superscripts $^{\text{in}}$ and $^{\text{out}}$ refer to flows/concentrations entering or leaving the unit, respectively; and $\rho_{k,c}$ stands for the removal efficiency of species c in unit k.

This latter removal efficiency is key to the accuracy of the superstructure optimization model, yet the direct use of complex biodegradation models (such as ADM1 [8] and ASM1-3 [32]) or complex crystallization/adsorption/filtration models in the MO-MINLP (P) is currently computationally intractable. As already mentioned, our approach considers surrogate models constructed from input-output data predicted by state-of-the-art process simulators instead. Specifically, the performance – either at steady state or averaged over a cyclic steady state – of a given unit can be computed for various influent compositions (COD, NH_4^+, etc) and given operation parameters (HRT, SRT, etc). Then, simple regression models can be fitted to the simulated data points, e.g. in the form of linear, piecewise-linear or polynomial input-output relationships, as appropriate. For instance, Fig. 1.2 shows the outlet COD concentration of an anaerobic digester predicted by the ManTIS3 model in GPS-X for various inlet COD and NH_4^+, along with the corresponding linear regression model used in the superstructure optimization problem (P). In order to limit the number of variables in the surrogate models, multiple instances of the same unit can be considered as part of the superstructure, which correspond to different sets of operating parameters; for example, two instances of an anaerobic digester with SRTs of 15 and 20 days.

1.3.3 ECONOMIC PERFORMANCE INDICATORS

The superstructure optimization problem (P) involves minimizing a number of KPIs representing a particular plant configuration's performance. As far as economical performance is concerned, one can consider the net present value (NPV) over the project's lifetime, given by:

$$\text{KPI}_{\text{NPV}} = -\text{CAPEX} + \sum_{yr=1}^{\text{LT}} \frac{(\text{SALES} - \text{OPEX})}{(1+\text{DISC})^{yr}}\,, \tag{1.1}$$

where LT denotes the project lifetime, typically 20 years; SALES represents revenues from energy/nutrient sales; CAPEX and OPEX denote the costs caused by WWTP capital investment and operation respectively; and DISC is the discount factor over the whole project lifetime, namely the rate at which future payoffs are discounted

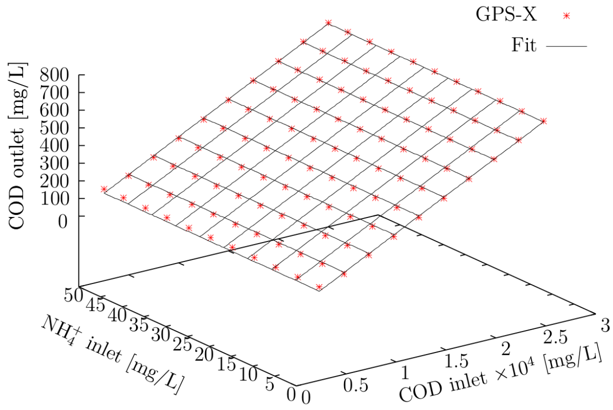

Figure 1.2 Illustration of a linear surrogate model obtained from GPS-X simulated data

back to present value. Alternatively, one may consider a life-cycle costing (LCC) indicator [63].

Reliable costing information needed to compute such indicators, including capital and operating costs, can be obtained from preliminary costing software, such as CapdetWorks®. The use of a common source and methodology for costing various technologies presents the advantage of consistency, although such data may not be widely available or reliable for the newer technologies. Similar to the approach outlined previously in Sect. 1.3.2 for plant-wide performance surrogates, one approach involves deriving costing surrogates based on data generated from these computer programs for each unit by varying their size and regressing these data as appropriate. Since the residence time in a given unit is fixed here, their volume is indeed proportional to the inlet flow rate.

1.3.4 ENVIRONMENTAL PERFORMANCE INDICATORS

The main environmental impacts associated with each process configuration in the superstructure can be estimated using LCA—an illustration of possible subprocesses modeled within the boundary of a WWTP system are shown in Fig. 1.3, which includes the WWTP infrastructure, operational inputs and emissions over the plant's lifetime. To carry out the inventory analysis, a rather natural choice for the functional unit is *'a unit volume of wastewater influent over a given time period'* [71]. Moreover, where a given product is attributed multiple functions, allocation can be made preferentially by substitution; for instance, treated effluents plus nutrients recovered from the WWTP would be accounted for as fertilizer replacement, and green electrical power generated from a CHP system would be exported to the grid. This way, a wastewater treatment facility is credited with the avoided environmental burdens, such as GHG emissions or resource depletion, that would otherwise be incurred by generating the corresponding amount of fertilizer or electricity through conventional routes.

Impact categories that are most relevant for wastewater treatment facilities include the global warming potential (GWP100) and the eutrophication potential (EP). The overall load for a given category j can be quantified as follows:

$$\mathrm{KPI}_j = \mathrm{INFRA}_j + \mathrm{LT} \cdot (\mathrm{OPER}_j + \mathrm{WWEFF}_j + \mathrm{WWSLU}_j - \mathrm{CRED}_j) \,, \tag{1.2}$$

where INFRA_j, OPER_j, WWEFF_j, WWSLU_j and CRED_j represent the individual loads associated with the required infrastructure, annual operation of the plant, discharged effluent, discharged sludge, and obtained credit, respectively. All these loads may themselves be computed as combinations of a list of 'elementary' environmental burdens corresponding, but not limited, to: the use of steel, concrete or electrical power; the emissions of CO_2 or methane from the treatment units; the release of COD, ammonia, phosphates or suspended solids with the treated effluent; and the utilization of nitrogen, phosphorus or magnesium resources. In particular, these elementary impacts can be obtained from the EcoInvent data base, which is available through LCA software such as SimaPro®. Aggregation of these various burdens into the loads in Eq. (1.2) relies on inventory data predicted by the plant-wide performance surrogates (Sect. 1.3.2). As a first approximation, the loads may be assumed to scale linearly with the inventory flows. Further details regarding the impact assessment can be found in [77, 59].

1.3.5 NUMERICAL SOLUTION STRATEGIES

The superstructure optimization problem (P) yields a nonconvex optimization model due to the presence of bilinear terms that arise in the material balances of the units as a result of contaminant mixing, in addition to other nonlinearities in certain performance and costing expressions. This nonconvexity can lead to multiple local optimal solutions, thereby calling for the implementation of global optimization techniques to guarantee a reliable solution. Recent work in water network synthesis [2, 38] demonstrates that deterministic global optimization solvers such as BARON [74] or ANTIGONE [55] are now able to provide global optimality certificates within reasonable computational times for such problems.

With regards to the multi-objective nature of the problem, popular (deterministic) approaches to computing Pareto sets include the weighted, ε-constraints and goal programming methods [62]. For instance, the weighted-sum approach combines a set of objectives into a unique objective by using weights which are varied in order to describe the solution set, whereas the ε-constraint method converts all but one objectives into inequality constraints whose right-hand-side values are varied to describe the solution set.

1.4 CASE STUDY

The main objective of the present case study is to illustrate the methodology outlined in Sect. 1.3, along with typical results. Due to space restrictions, the reader is referred to [77, 59] for a more detailed account of the results and further discussion.

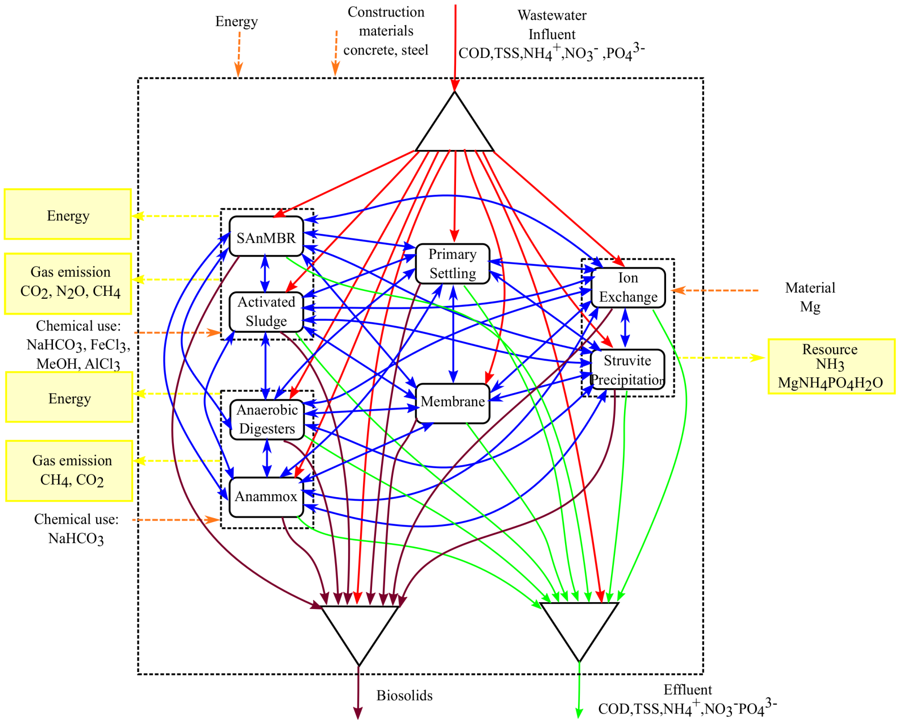

Figure 1.3 Schematic representation of the system boundary and superstructure in the case study [59]

The case study considers the synthesis of a wastewater treatment/recovery facility for a 10,000 m^3/day municipal wastewater stream with the average compositions reported in Table 1.1. In agreement with the EU Directive 91/271/EEC on Urban Wastewater Treatment, the targeted maximum concentrations for the treated effluent stream are 142.3 mg/L total COD, 7.6 mg/L NH_4^+, 10.3 mg/L NO_3^-, 0.82 mg/L PO_4^{3-} and 25.9 mg/L TSS, which correspond to minimum abatements of 75% total COD, 80% total N and total P, and 90% TSS. Besides the inlet and outlet wastewater streams, the case study also considers an outlet biosolids stream in connection to sludge production. The superstructure shown in Fig. 1.3 is comprised of the following treatment/separation units—see [60, 77] for further details:

- *Biological treatment*, including 3 activated sludge processes (with i. nitrification, ii. nitrification and denitrification, and iii. enhanced phosphorus removal), 1 SAnMBR unit, 2 digesters (with solids retention times of 15 and 20 days), and 1 Sharon-Anammox Process;
- *Resource recovery*, including 1 struvite precipitation unit for P recovery and 1 ion exchange unit for N recovery;
- *Physical separation*, with 1 membrane unit, and 1 primary clarifier (besides

the secondary clarifiers of the activated sludge processes).

The focus is on optimizing two KPIs, namely NPV and GWP100 over a period of 20 years.

In order to carry out the computations, the performance of each treatment unit is predicted by the ManTIS3 simulator within GPS-X®, which includes the most common biological, physical and chemical processes in WWTPs. Surrogate models are developed for the biological treatment units based on performance and GHG emission projections by the simulator. For the membrane units and the primary clarifier, simple models based on split fractions for the solids are used, assuming no biological reactions and a perfect split for the soluble species. Finally, performance predictions for the ion exchange units are based on literature data, regressed by the Langmuir isotherm model [60, 77]. In addition, the CAPEX and OPEX of all the units, but membranes, are estimated using CapdetWorks™, and regressed with simple linear models as a function of the unit volume and/or processed flow rate (within the operational range). The CAPEX and OPEX of the membrane units, on the other hand, are set based on expert's recommendations [60]. The LCA model is implemented in Simapro 7.3, with a midpoint approach CML 2 baseline 2000 (V2.05) applied as characterization method at the LCIA stage. Statistics on the UK country-level N and P fertilizer composition (International Fertilizer Industry Association 2014) and UK average electricity grid mix [19] are adopted in this study to credit the WWTP system with the avoided production of fertilizers and electricity. The inventory for generic fertilizer production and fuel combustion is derived from the EcoInvent database (v2.2).

Table 1.1
Composition of the municipal wastewater in the case study

Total COD	Soluble COD	TSS	VSS	VFA
569 mg L^{-1}	129 mg L^{-1}	259 mg L^{-1}	231 mg L^{-1}	10 mg L^{-1}
Total N	**Ammonia**	**Total P**	**Phosphate**	**Alkalinity**
51.6 mg L^{-1}	38 mg L^{-1}	7.6 mg L^{-1}	4.1 mg L^{-1}	253 mg $CaCO_3$ L^{-1}

The optimal configuration shown in Fig. 1.4 is obtained by maximizing the NPV of the treatment facility only, without consideration to environmental impacts; that is, it corresponds to one of the end-points of the Pareto set (single-objective optimization). About 91% of the wastewater stream is processed in the activated sludge process with enhanced phosphorus removal (A2O), before mixing with the remaining part of the wastewater stream and discharging into the environment. The sludge produced by the activated sludge treatment is processed into the anaerobic digester

(SRT 20 days), whose supernatant stream is returned to the activated sludge unit and the biosolids stream is disposed into a landfill. The treated wastewater meets all the discharge requirements, and it is the minimum TSS abatement of 90% which happens to be the most restrictive here. The NPV for this optimal configuration is estimated as M£-7.69, with the breakdown costing analysis including CAPEX, OPEX and SALES shown in Table 1.2. Because CAPEX is indeed the largest contributor to NPV, the WWTP configuration for maximizing NPV is comprised of a minimal number of treatment units in order to comply with the discharge constraints. Moreover, a longer SRT is selected for the anaerobic digester in order to increase the amount of biogas produced and mitigate the sludge disposal cost.

Table 1.2
Economic and environmental performance in the case study problems

Flowsheet	maximal NPV	maximal enviroeconomic value
CAPEX, M£	-5.42	-7.70
OPEX, M£/yr	-0.45	-0.64
SALES, M£/yr	0.24	0.42
NPV, M£	-7.69	-10.07
GWP100, $\times 10^4$ tCO_2e	23.2	1.72
Net profit, M£	-14.3	-10.6

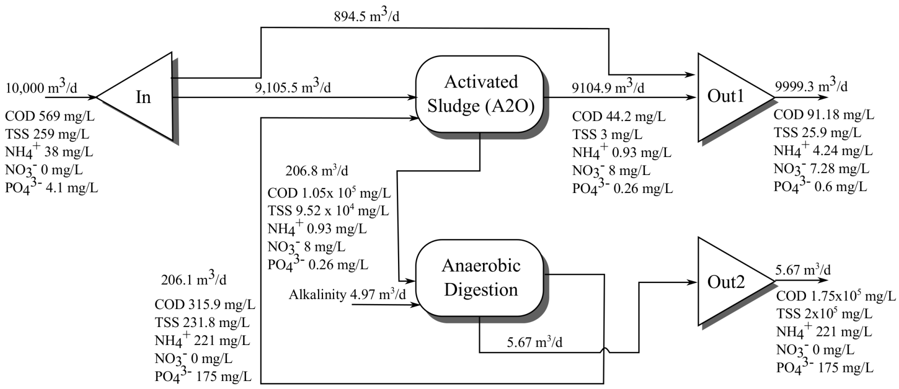

Figure 1.4 Optimal plant configuration for the NPV maximization problem

In the enviroeconomic optimization problem, the conflicting objectives of NPV and GWP100 are considered simultaneously. The plant configuration shown in Fig. 1.5 is one particular point on the optimal Pareto solution set (not shown); if monetization were used for GWP100, this solution would correspond to a carbon trading price of £28.5/tCO_2, currently DECC's central scenario [18]. Observe that this plant configuration is markedly different from the economically optimum one in Fig. 1.4. The SAnMBR unit treats about 96% of the incoming wastewater stream: the sludge produced by this unit is processed in the anaerobic digester (SRT 20 days), whose digester cake is sent for disposal, incurring a significant cost due to the landfill tax. Furthermore, the digester liquor is mixed with both the SAnMBR outlet stream and the bypass stream, and passed through the ion exchange and struvite precipitation units for N and P recovery. Here again, the treated wastewater meets all the discharge requirements, but it is now the minimum phosphate abatement of 80% which becomes most restrictive. As shown in Table 1.2, the NPV is greater by about M£2.4 due to a high CAPEX, but the GHG emissions are reduced by over 13 fold, thus defining an enviroeconomic trade-off. The SAnMBR unit becomes part of the optimal configuration in combination with both N and P recovery units due to their lower GHG emissions compared with conventional activated sludge treatment, both CO_2 emissions from electrical power consumption and N_2O evolved from biological nitrification/denitrification.

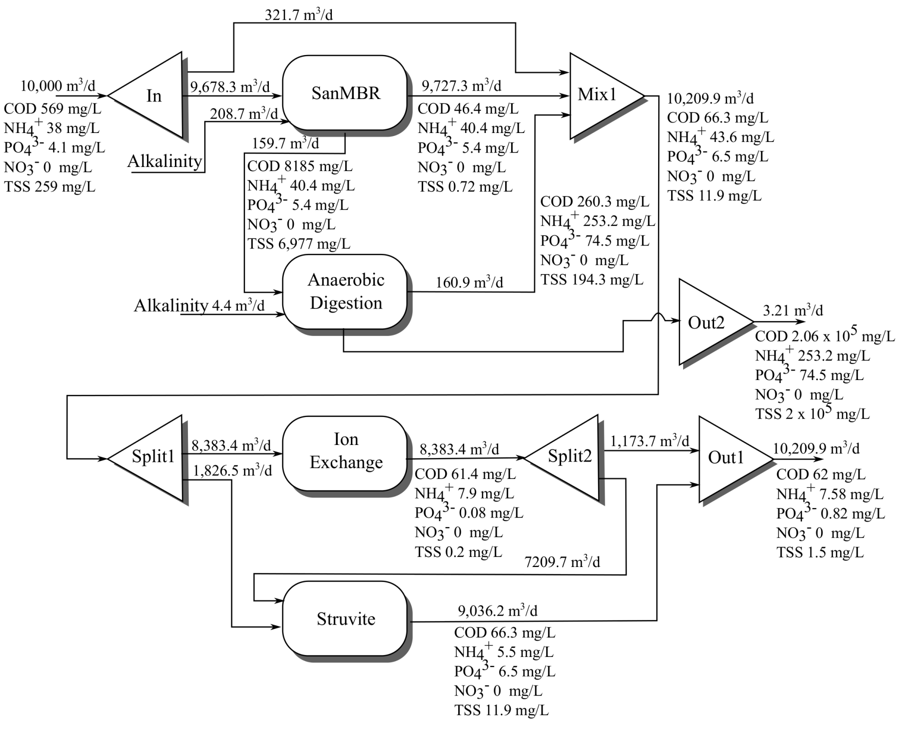

Figure 1.5 Optimal plant configuration for the enviroeconomic optimization problem

1.5 CONCLUSIONS

This chapter has presented and illustrated a systematic optimization-based methodology for incorporating LCA alongside economic criteria into a multi-objective optimization methodology for the synthesis of sustainable WWTPs. This methodology relies on surrogate models as a means for overcoming the limitation of current global optimization technology, which does not allow for optimizing complex plant configurations (e.g., complex biological processes, multiple scales, time dependence, etc) all in a single step. A key requirement in applying this methodology nonetheless is the availability of reliable performance models for the treatment and separation units, on the one hand, and reliable costing and environmental impact data, on the other hand. Our work advocates the use of state-of-the-art wastewater treatment simulators for deriving simple response-surface models, which are general enough to be independent of detailed design choices and keep the superstructure optimization model computationally tractable; and the use of LCA state-of-the-art databases to assess the main environmental impacts likewise.

Overall, this methodology should be regarded as a decision-support system for identifying, among hundreds or even thousands of alternatives, a number of promising wastewater treatment and resource recovery systems for a given wastewater stream and regional context. The preselected plant configurations can be considered for detailed design analysis and optimization in a subsequent step. The case study results demonstrate that the proposed framework can provide valuable insights for decision-making in WWTP design (see also [77, 59]), and that LCA integration into decision-making tools for wastewater treatment alongside economical considerations may lead to radical changes in the design of tomorrow's wastewater treatment facilities.

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