Optimization-based Methodology for the Development of Wastewater Facilities for Energy and Nutrient Recovery

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Abstract

A paradigm shift is currently underway from an attitude that considers wastewater streams as a waste to be treated, to a proactive interest in recovering materials and energy from these streams. This paper is concerned with the development and application of a systematic, model-based methodology for the development of wastewater resource recovery systems that are both economically attractive and sustainable. With the array of available treatment and recovery options growing steadily, a superstructure modelling approach based on rigorous mathematical optimization appears to be a natural approach for tackling these problems. The development of reliable, yet simple, performance and cost models is a key issue with this approach in order to allow for a reliable solution based on global optimization. We argue that commercial wastewater simulators can be used to derive such models, and we illustrate this approach with a simple resource recovery system. The results show that the proposed methodology is computationally tractable, thereby supporting its application as a decision support system for selection of promising resource recovery systems whose development is worth pursuing.

Keywords: biological treatment, biorefining, energy recovery, nutrient recovery, superstructure optimization, wastewater treatment

1. Introduction

For a long time wastewater has been considered a human health concern and environmental hazard. For the most part, wastewater treatment design retains its

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foundations in engineering traditions established back in the early 20th century (Daigger, 2009). To produce an effluent that was of satisfactory quality for discharge into the environment, processes were developed which used large amounts of energy and land, and produced large amounts of sludge. However, a paradigm shift is underway towards making wastewater treatment facilities more sustainable. 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* (Guest et al., 2009). It has even been argued that the design of wastewater facilities could have a significant impact on greenhouse gas emissions (Bufe, 2008).

Until recently a majority of the activities related to resource recovery from wastewater have focused on waste sludge streams, which are a by-product of biological treatment. Because these streams have relatively low flows in comparison to the main wastewater stream, and are more concentrated, resources can be recovered from them with minimal changes to the wastewater treatment infrastructure. For instance, mesophilic anaerobic digestion of primary and waste-activated sludge produces a methane-rich gas which is being used in most treatment facilities worldwide to recover energy. It has been reported that a quarter to half of the energy requirements for an activated sludge facility can be provided by such energy recovery systems (Crawford & Sandino, 2010; McCarty et al., 2011), and these figures keep increasing as new practices and technologies are being deployed. A recent review of the current opportunities for resource extraction from sludge streams—both energy and materials—was conducted by Hydromantis Inc. (2008).

The main focus of this paper is on direct resource recovery from municipal and industrial wastewater—although it should be stressed that this methodology can also be extended to encompass wastewater sludge as well. A diverse toolkit is available and is increasingly being applied by practitioners to promote sustainability. The recovery of water as a resource, known as water reclamation and reuse, is an established practice (Tchobanoglous et al., 2003). Municipal water reuse is practiced widely in water-short locations, to meet agricultural, industrial, and urban irrigation water needs; domestic water reuse, although less practiced, is also increasing (Daigger, 2009). In this work, we are addressing applications where, in combination with the production of water suitable for reuse, other resources are recovered from the wastewater.

The increasing market value of wastewater components, such as ammonia and phosphorus, are acting as key drivers for resource recovery from wastewater. Because phosphorus is mined as a mineral, and thus is a limited resource, its commercial value will inevitably increase as it is depleted (Bufe, 2009; Mihelcic et al., 2011). The production of ammonia, on the other hand, has a substantial energy requirement and concomitant Greenhouse Gas (GHG) emission (Galloway & Cowling, 2002), and hence its price is increasing with energy costs. Besides nutrients, organic carbon can be recovered from wastewater using anaerobic digestion to produce a methane-rich biogas (Jeison & van Lier, 2008) that can be combusted on-site for heat or electricity generation, or cleaned-up and sold. Other examples of newer technologies for carbon recovery include microbial fuel cells (Logan et al., 2006) as well as the production of bioplastics (Coats et al., 2007). This potential for water, materials and energy recovery has also attracted a lot of interest from industry (see, e.g., Veolia Environment, 2010).

There seems to be a general consensus that wastewater (and wastewater sludge) is a potential source of valuable resources, and that the technology needed for such resource recovery is maturing. Besides the technological and market penetration barriers, the lack of decision-making tools and design methodologies remains a major problem to identifying the most sustainable solutions in a given geographic and cultural context (Guest et al., 2009; Parker, 2009). Such decisions need to be made by considering whether a resource recovery facility will have a net positive impact in terms of a number of economic, environmental and socio-cultural criteria. These types of decisions are typically comparative in nature, and can take advantage of life cycle analysis (LCA) or triple bottom line (3BL) techniques to make quantitative assessments.

Nevertheless, as the array of technical options grows, a simple enumeration of all possible alternatives quickly becomes unmanageable, let alone the fact that each technology has its own parameters to specify or optimize. In this paper, we advocate the use of systems engineering methods and tools to address this problem in a systematic way. A superstructure modelling approach (Bielger et al., 1997) is considered which can account for a large number of treatment and separation options (units) along with all feasible interconnections between them. Rigorous optimization based on such a superstructure leads to mixed-integer nonlinear programs (MINLPs) that can be implemented and solved using state-of-the-art mathematical optimization software such as GAMS (`http://www.gams.com`). However, key to the success of this methodology is the development/selection of mathematical models for the units that are simple enough for the optimization problem to remain tractable, yet provide reliable estimates of their performance and associated costs.

In the remainder of this paper we will review the main resource recovery options from wastewater in Sect. 2. We will then describe the superstructure optimization approach in Sect. 3, with emphasis on performance models for the units and assessment criteria. This approach is illustrated by the synthesis of a simple resource recovery facility in Sect. 4. Finally, we conclude the paper with a general discussion of the ensuing challenges and opportunities.

2. Resource Recovery from Wastewater

State-of-the-art wastewater treatment facilities are designed to remove substances that are considered as contaminants, rather than as resources. One striking example of this is the characterization of organic carbon compounds in terms of their (bio)chemical oxygen demand (BOD/COD), making it clear that such compounds are undesirable. Nitrogenous and phosphorous compounds too are transformed or removed due to their potential to trigger eutrophication (both N and P) or their aquatic toxicity (ammonia). Moreover, the removal of carbon-, nitrogen- and phosphorous-bearing compounds not only requires energy and/or chemicals, but it often yields byproducts, typically of limited value and often requiring further processing. The remainder of this section reviews a number of promising technologies that are being developed for recovery of energy and materials from wastewater; the emphasis is on proven technologies.

2.1. Energy Recovery

The organic compounds present in municipal (and many industrial) wastewaters can be converted into a methane-rich biogas via anaerobic digestion. A quick calculation suggests that about 30-60 L/day of methane per capita could be generated from typical municipal wastewater if all the biodegradable organic matter were transformed into biogas, in addition to removing the extra costs for aeration associated with conventional activated sludge processes (Owen, 1982). Moreover, anaerobic digestion has little effect on ammonia or phosphates, and therefore it is a perfect match for resource recovery where nutrients can be separated from the effluent in downstream units.

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 15°C. Innovations in reactor design to maintain elevated biomass inventories, such as upflow anaerobic sludge blanket (UASB) and anaerobic membrane bioreactor (AnMBR), have mitigated some of the limitations and extended the range of applications of anaerobic treatment (Liao et al., 2006; Lew et al., 2009). Particularly promising configurations include the submerged anaerobic membrane bioreactor (SAnMBR; Hu & Stuckey, 2006; Lin et al., 2012) and, more recently, the anaerobic fluidized membrane bioreactor (AFMBR; Kim et al., 2011). Research is underway to develop improved membranes and reactor designs that reduce membrane fouling and enhance dissolved methane recovery (Stuckey, 2012; Smith et al., 2012).

In those urban water systems where heat accumulates in the wastewater, 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 can be suitable, e.g., for heating buildings (EPA, 2007). Besides biogas and thermal energy, newer technologies that try to generate electricity or hydrogen from wastewater are also worth mentionning (Logan et al., 2006; Kim & Logan, 2011).

2.2. Materials Recovery

Recent spikes in the price of mineral phosphorus (P) is making P recovery an increasingly economically attractive option. In the absence of a precipitating or fixing agent, a majority of the phosphates (PO_4^{3-})—between 50-80% of the total phosphorous compounds in municipal wastewater are phosphates (Tchobanoglous et al., 2003)—will leave with the 'treated' effluent at a wastewater facility, from where they can be recovered. Nitrogenous (N) compounds, on the other hand, can be generated from atmospheric nitrogen and are not a limited resource, albeit their production is an energy-intensive process. With increasing energy costs, N recovery from wastewater effluents—between 50-80% of total nitrogen present in municipal wastewater is soluble and a majority is released in inorganic form (Tchobanoglous et al., 2003)—is also becoming economically viable.

Either ammonia, nitrate or phosphates can be recovered by passing the secondary effluent through adsorbent ion exchange columns (Liberti et al., 2001; Johir et al., 2011). The columns need to be regenerated cyclically by desorbing both N and P, usually with a low volume, concentrated brine solution. The resulting N-and P-enriched solutions can then be mixed and further processed into a saleable product (e.g. fertilizer, see below). Ion exchange presents the additional advantage that N and P recovery can be achieved over a wide range of temperatures that are challenging for biological removal processes. Nonetheless, some of the challenges associated with the use of ion exchange include the potential for fouling with suspended solids, the limited exchange capacity of certain adsorbents which require regeneration every few hours, the limited selectivity due to ion competition for the resin sites, and the large capital cost (Miladinovic & Weatherley, 2008). The use of natural zeolites (e.g. clinoptilolite) to adsorb ammonium ions (NH_4^+) from wastewater has received considerable attention (Aiyuk et al., 2004; Wang & Peng, 2010), and more recently polymeric resins that have higher exchange capacities than zeolites. Research is also underway to develop anion adsorbents with high phosphate selectively and easy regeneration characteristics, including hydrotalcite (HTAL) (Kuzawa et al., 2006) and polymeric resins with hydrated ferric oxide nanoparticles (Martin et al., 2009).

An attractive alternative to ion exchange 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. For instance, continuous backwash filters made of hydrous ferric oxide (HFO) coated sand, where continuous regeneration is accomplished by adding 5-10 mg/L of ferric chloride ($FeCl_3$), have been reported to achieve up to 95% P removal from secondary municipal effluents (Newcombe et al., 2008). In these processes, P recovery can be simply achieved with a membrane separator receiving the backwash from the reactive filter (Sutton et al., 2011), although further processing is then needed to convert P into a saleable product.

Another technology that has gained substantial interest to help recover phosphorus from concentrated wastewater streams is crystallization into reusable compounds such as calcium phosphate ($Ca_3(PO_4)_2$) and struvite ($MgNH_4PO_4$) (Le Corre et al., 2009). Although both can be used in agriculture as fertilizers, struvite is preferred due to the fact that magnesium (Mg), N and P are released simultaneously (1:1:1 molar ratio), and that the rate of nutrient release is slower compared to other fertilizers. The recovery technology involves precipitation in either stirred tank or fluidized bed reactors (Bhuiyan et al., 2008), the latter being the most commonly used to crystallize struvite from wastewater. Most applications to date have used sludge liquors generated from anaerobic digesters as their influent streams, with phosphate concentrations in the range 50-100 mg/L; removal efficiencies of 80% or higher have been reported under well-controlled conditions (Ueno & Fujii, 2001). For more dilute streams, such as secondary effluents with phosphate concentrations in the range 4-12 mg/L, struvite crystallization can be combined with adsorbent columns and fed with the enriched solutions from the adsorbent regeneration; the RIM-NUT® process by Liberti et al. (2001) applies this strategy.

Besides nutrients, organic carbon (OC) recovery can be achieved via the production of polyhydroalkanoates (PHAs), a precursor of bioplastics (Coats et al., 2007). PHAs are linear polyesters produced from the fermentation of sugars or lipids by bacteria as energy storage (up to 50% weight). Their production is technologically proven from synthetic wastewater and under well-controlled conditions. However, full-scale applications are still at the embryonic stage, in part due to the challenge associated with the separation of PHAs from the bacterial biomass. It should also be clear that PHA production, when used in combination with anaerobic digestion, will result in a net reduction of biogas production by the digester since it diverts part of the available OC.

Other materials recovery concern heavy metals, for which many separation technologies have been proposed including, but not limited to, ion exchange, adsorption, membrane filtration, and chemical precipitation (Fu & Wang, 2011).

3. Development of Resource Recovery Facilities

The combination of traditional wastewater treatment technology with 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.

Recently, Sutton et al. (2011) developed a wastewater process concept that integrates biological processing with physical and chemical separation units for the conversion of OC to methane, the recovery of P and N, and the production of water suitable for reuse. More generally, this raises 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—this problem is known as *synthesis* or *flowsheeting* in process engineering.

For the synthesis of sustainable resource recovery facilities from wastewater, one must account for the trade-offs between capital and operating costs and sales on the one hand, and water quality and other environmental considerations on the other hand. While technical insights can significantly reduce the combinatorial problem and often allow us to arrive at promising solutions, as in Sutton et al. (2011), they do not always provide all the information that is required for an optimal (or near optimal) system. In general, one may still be left with the problem of having to search among a relatively large number of alternatives, thereby calling for systematic optimization based on a superstructure representation.

3.1. Superstructure Representation

Systematic methods for the synthesis of complex chemical plants and biorefineries, based on superstructure modeling and optimization, are well developed (Bielger et al., 1997; Kokossis & Yang, 2010; Liu et al., 2011). 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 and recycle/reuse (Faria & Bagajewicz, 2009; Khor et al., 2012). In contrast, as far as municipal wastewater facilities are concerned, only limited work has been reported to date (Rigopoulos & Linke, 2002; Alasino et al., 2007), although the need for systematic approaches was emphasized, e.g., in Balkema et al. (2001) and Hamouda et al. (2009).

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 from local regulations;
- a set of treatment and separation units with given performance for target compounds.

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, for a simple network topology that consists of a single wastewater stream, a single water sink, and six treatment/separation units.

[Figure 1 about here.]

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.

- The optimal system configuration is one that maximizes a certain sustainability index of the facility, for instance a weighted sum of LCA impacts (Corominas et al., 2013). Alternatively, one can choose to maximize the economic efficiency of a facility, e.g. using life-cycle costing (LCC; Rebitzer et al., 2003) or simply in terms of its net present value (NPV) over the project lifetime:

  $$\mathrm{NPV} = -\mathrm{CAPEX} + \sum_{\mathrm{yr}=1}^{\mathrm{lifetime}} \frac{\mathrm{SALES} - \mathrm{OPEX}}{(1 + \mathrm{DISCOUNT\_RATE})^{\mathrm{yr}}}, \tag{1}$$

  where SALES stands for revenues from energy/product sales.
- Regarding constraints, material balances on flows (F) and concentrations (X) around the sources, the units, and the sinks are to be obeyed in addition to the discharge limits and certain design and structural specifications. For instance, the material balances around a given treatment unit k for a species c can be written as:

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

where the superscrits $^{\text{in}}$ and $^{\text{out}}$ refer to flows/concentrations entering or leaving the unit, respectively; and ρ stands for the removal efficiency in the unit. In turn, discharge limits ($X^{\max}$) can be enforced on a given sink j for a species c as:

$$
\sum_{i=1}^{N_{\text{source}}} F_{i\to j}\, X_{i,c} + \sum_{k=1}^{N_{\text{unit}}} F_{k\to j}\, X_{k,c}^{\text{out}} \leq X_{j,c}^{\max}\ .
$$

Key to the accuracy of such a superstructure representation are the performance and costing models used to populate the objective and constraint functions, as discussed next.

3.2. Performance Models and Costing of the Units

The aim of a wastewater/resource recovery facility is to remove and recover contaminants from the effluent and generate energy, and it is the role of the mathematical models of each treatment/separation unit to predict their performance. To comply with the superstructure optimization approach and the current capabilities of optimization technology, however, these models must remain as simple as possible, typically linear, piecewise-linear or polynomial relationships between the input/output variables. Needless to say, direct use of complex biodegradation models such as ADM1 (Batstone et al., 2002) and ASM1-3 (Henze et al., 2007) for the bioreactors or complex crystallization, adsorption and filtration models for the separation units in the superstructure for performance prediction is currently intractable from a computational standpoint.

[Figure 2 about here.]

In this context, one simple approach consists in assuming fixed conversion, removal or split ratios in the treatment and separation units. This is the approach typically used in water network synthesis problems (see, e.g., Khor et al., 2012). In this work, we advocate an alternative, potentially more accurate, approach that relies on detailed first principle models, as implemented in wastewater treatment simulators such as GPS-X$^{\text{TM}}$ (Hydromantis Inc., 2011b). Based on the average performance predicted by a simulator—either at steady state or averaged over a cyclic steady state—for various influent compositions (COD, TSS, *etc*) and given operation parameters (HRT, SRT, *etc*), simple regression models can be fitted to the simulated data points. Fig. 2 shows an example of methane conversion efficiency in a UASB reactor as predicted by the ManTIS2 model in GPS-X$^{\text{TM}}$ for various HRTs, along with a corresponding piecewise-linear regression model for use in the superstructure model.

Similarly, reliable costing information—both capital and operating costs—can be obtained from preliminary costing software, such as CAPDETWORKS$^{\text{TM}}$ (Hydromantis Inc., 2011a). Here again, data can be generated by such programs for various unit volumes and/or flowrates and regressed to yield simple linear, piecewise-linear or polynomial models. Using a common source and methodology for costing various technologies is clearly advantageous with regards to consistency.

3.3. Numerical Solution Strategy

In optimizing a superstructure for synthesizing a resource recovery system, the optimization model will contain 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 composition as well as certain design and operating parameters, here denoted by x.

Such an optimization can be posed as the following mathematical programming problem:

$$\begin{aligned} \min_{x,y} \quad & f(x,y) \\ \text{s.t.} \quad & h(x) = 0 \\ & g(x,y) \leq 0 \\ & x \leq 0, \;\; y \in \{0,1\}. \end{aligned} \tag{P}$$

The objective function $f(x,y)$ in (P), which either expresses a sustainability or economic index (see Sect. 3.1), is a function of both types of variables. The continuous variables x, which for physical reasons are assumed to be non-negative, must obey material balance equations of the form $h(x) = 0$ (see Sect. 3.2), where usually $\dim(h) < \dim(x)$. Both continuous and binary variables must also satisfy the design specifications in terms of discharge allowance and physical operating limits, as well as logical constraints such as the existence of piping interconnections for nonzero flows or to enforce the sequencing of certain units. A detailed formulation of the optimization model can be found in Gomes-Mont (2011).

The superstructure optimization model (P) yields a nonconvex MINLP problem 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 the performance and costing expressions. Such nonconvexity can result in multiple local optimal solutions, thereby calling for the implementation of global optimization techniques to guarantee a reliable solution. Fortunately, recent work in water network synthesis (Ahmetović & Grossmann, 2011; Khor et al., 2012) demonstrates that deterministic global optimization solvers such as BARON (Tawarmalani & Sahinidis, 2004) are now able to solve such problems with reasonable run times to global optimality. Moreover, the situation is improving as new solvers such as GloMIQO (Misener & Floudas, 2013) are becoming available.

3.4. Superstructure-based Optimization Methodology

Superstructure modelling and optimization is at the core of the synthesis of sustainable resource recovery facilities. In an overall design methodology (Fig. 3, the most promising alternatives would in turn be validated against the performance and cost predicted by the wastewater treatment simulator. Typically, this would create an iteration between the superstructure optimization and the simulator in order to refine the regression models as appropriate. In particular, recent developments in surrogate-based optimization can guarantee to the overall optimum with minimum recourse to detailled models (Agarwal & Biegler, 2013; Biegler et al., 2014). Finally, the selected process candidates would be considered for detailed performance and cost analysis, including integration options and operability issues. Here again, further iterations with the superstructure optimization block could prove necessary in order to account for additional design and operational constraints.

[Figure 3 about here.]

The focus in this paper is more specifically on the components in the grey-shaded area of Fig. 3. The main objective of the following case study is to provide a proof-of-concept of this superstructure optimization approach based on simple regression models, also showing that the underlying optimization problems are indeed tractable to guaranteed global optimality.

4. Case Study

We consider the synthesis of a resource recovery facility for the treatment of 100 m^3/h of an industrial wine distillery effluent, whose average composition for the main species is given in Table 1 (Melamane et al., 2007). The objective is to maximize the NPV given in Eq. (1), while satisfying maximum discharge requirements as defined by the EU Directive 91/271/EEC on Urban Wastewater Treatment; these requirements consist of meeting either minimum abatements of 75% total COD, 80% total N and total P, and 90% TSS, or maximum concentrations of

10 g/L total COD, 0.4 g/L total N, 0.07 g/L total P, and 0.5 g/L TSS—but not necessarily both.

[Table 1 about here.]

A small superstructure that consists of 2 biological treatment units (UASB, SMBR), 2 filtration units (sand filter, membrane unit), and 2 nutrient recovery units (struvite crystallizer, zeolite adsorber) is investigated. This problem is kept relatively simple as the main objective of the case study is to assess the proposed optimization methodology. More challenging problems that include a variety of treatment/recovery options for carbon, nitrogen and phosphorus are beyond the scope of this paper and will be investigated as part of future work.

- The performance of the UASB and the SMBR are approximated based on the ManTIS2 and ASM1 models in GPS-X$^{\text{TM}}$, respectively. The degradation rates of total COD, total N, ammonia, total P, phosphate, and TSS, as well as the production rate of methane in a UASB, are regressed using either linear or piecewise-linear models within an HRT range of 2-20 day^{-1}. A subset of such performance models are shown in Figure 4 (left and centre plots) for a UASB unit.

[Figure 4 about here.]

- The performance of the filtration, membrane and struvite units is also predicted by using simple models in GPS-X$^{\text{TM}}$, and then averaged to yield constant removal/conversion efficiencies as a first approximation. The zeolite (ion exchange) unit, currently unavailable in GPS-X$^{\text{TM}}$, is also approximated using constant efficiencies gathered from the literature (Gomes-Mont, 2011).

- The CAPEX and OPEX of all the units, with the exception of the membrane unit, are estimated using CapdetWorks$^{\text{TM}}$, and then regressed with simple linear models as a function of the unit volume and/or processed flow rate in the range of operation. This is illustrated in Figure 4 (right plots) for the CAPEX and OPEX of a UASB unit. For the membrane unit, currently unavailable in CapdetWorks™, rough estimates of the CAPEX and OPEX were used as recommended by membrane experts (Judd, 2012).

- Besides the treatment/separation units in the superstructure, an auxiliary piece of equipment is the electricity generator from biogas. This technology is well developed, with companies such as Alstom, Capston or General Electric providing lines of engines specially adapted for biogas from anaerobic digestion. An average conversion efficiency of 40% is assumed here for the generator, and the OPEX and CAPEX are estimated based on data published by the United Nations Framework Convention on Climate Change (UNFCCC) and the International Energy Agency (IEA); see Gomes-Mont (2011) for details.

[Figure 5 about here.]

A constraint regarding the interconnections in the superstructure is that the effluent from the UASB must pass either through the sand filter or through the membrane unit before it can be sent to the zeolite and/or struvite units for nutrient recovery; this is to prevent large concentrations of solids in the latter. The computed optimal structure is displayed in the top part of Figure 5—Flowsheet A. The wastewater stream is first split in such a way that about 60% is processed in the UASB, before passing through the sand filter together with the remaining 40% of the raw wastewater stream. The sand filter outlet is then passed successively through the ion exchange column and the struvite crystallizer for nutrient recovery. While the effluent satisfies all of the discharge requirements, it is the minimum abatement of 80% in total P which turns out to be the most restrictive here. Moreover, a majority of the residual COD concentration is comprised of non-biodegradable soluble compounds, the other part being biodegradable soluble compounds from the wastewater fraction not treated in the UASB.

An NPV of about -7.68 M$ is found for this flowsheet over a period of 20 years, and the breakdown of these costs in terms of CAPEX, OPEX and SALES is given in Table 2. This negative NPV is mainly due to the rather large CAPEX—more than 40% incurred by the UASB unit, which cannot be offset by the net annual profit of about 0.88 M$, although the sales revenue, mainly electrical power from biogas combustion, exceeds the OPEX. Therefore, while such a resource recovery facility may not completely offset the infrastructure and operating costs solely based on electricity and nutrient sales, it would greatly mitigate the cost of wastewater treatment to comply with the discharge regulations.

[Table 2 about here.]

The decision to split the wastewater stream and not to process around 40% of that stream in the UASB unit may first appear counter-intuitive given the fact that most of the sales revenue is from the biogas produced in the UASB. However, in terms of the NPV, producing more biogas is only justified when the added sales revenue can offset the extra CAPEX and OPEX for a bigger UASB unit; this condition is not met in the present case study, and it would be worth investigating the sensitivity of this trade-off further to validate this finding.

To confirm this trend, we considered removing the possibility of bypassing the UASB by sending part of the wastewater stream directly to the filtration units. The resulting superstructure is depicted in the middle part of Figure 5—Flowsheet B. In this second flowsheet, a small part of the wastewater stream is now mixed directly with the treated effluent stream, without being processed. As expected the estimated NPV value of Flowsheet B decreases compared to Flowsheet A—see Table 2 for a break-down. In particular, this is a rather large decrease of about 3 M$. Finally, preventing part of the wastewater stream to be directly mixed with the treated effluent leads to the superstructure depicted in the bottom part of Figure 5—Flowsheet C. The estimated NPV of this third flowsheet turns out to be comparable with the estimated NPV of Flowsheet B.

Future investigations around this case study will aim at extending the set of treatment/recovery options in the superstructure, including anammox for ammonia removal or adsorptive phosphorous removal. The possibility of having multiple treatment stages, e.g., for the sand filtration units, will also be investigated in order to yield more efficient wastewater facilities, as well as for coping with more stringent effluent regulations.

5. Conclusions and Future Directions

In this paper, a systematic optimization-based methodology for the synthesis of wastewater/resource recovery facilities has been discussed and illustrated with a case study. By and large, this methodology should be regarded as a decision support system for isolating, among hundreds or even thousands of alternatives, those promising resource recovery systems whose development is worth pursuing. Based on this preselection, further simulation and optimization studies can then be undertaken to refine the performance and cost prediction by taking into account detailed design and operation considerations, as well as process integration. Such decomposition is indeed warranted as current computational capabilities and available algorithms do not allow for the optimal design and operation to be solved in a single step due to complex unit configuration, multiple scales, time dependence, and uncertainty.

A major hurdle in applying this methodology appears to be the availability of reliable performance models for the treatment and separation units as well as reliable (capital and operation) costing data. Here, we advocate the use of state-of-the-art wastewater treatment simulators in order to derive simple response-surface models, which are general enough to be independent of detailed design choices and keep the superstructure optimization model computationally tractable—this approach was demonstrated on a simple case study. Naturally, such simple models carry significant uncertainty and usually only provide a rough approximation of the actual performance of such complex units. A way to refine these models involves performing an iteration between the detailed process simulators and the superstructure optimization problem. Moreover, for those treatment/recovery techniques that are are less well established or lack reliable performance models, a scenario-based analysis can be applied, whereby multiple sets of resource recovery systems are determined on account of the forecast performance and cost scenarios. In particular, this analysis can be useful for resource allocation, for instance to help determine which technologies are critical and focus further research and development effort.

As for future research directions, a key extension will be to integrate wastewater and biosolids management within the same recovery system. Another important research activity should be the development and regular update of information databases as new advanced treatment and recovery technologies develop, or as the economic, environmental and socio-cultural contexts evolve. Besides the availability of feasible technologies that can transform wastewater into a product, and the downstream processing of this product into a saleable item, the circumstances that are required to successfully establish a functioning and sustainable resource recovery system also involves developing a distribution infrastructure and catching investors' interest in developing such technologies.

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Table 1: Characteristics of the industrial wine distillery wastewater

Total COD	Soluble COD	VFA	TSS	VSS
40 g/L	16 g/L	4.8 g/L	5 g/L	2.8 g/L
Total N	Ammonia	Total P	Phosphates	Alkalinity
2 g/L	0.14 g/L	0.35 g/L	0.16 g/L	3100 meq/L

Table 2: Cost analysis for the case study. A: No further restrictions on the interconnections; B: Bypass from source to sand filter not allowed; C: Bypass from source to sand filter or source to sink not allowed.

Flowsheet	A	B	C
CAPEX [M$]	**18.70**	**27.85**	**28.25**
UASB	41.2%	54.1%	54.2%
Electicity Generator	14.4%	16.4%	16.4%
Sand Filter	14.1%	9.4%	9.3%
Struvite Crystalizer	13.2%	8.8%	8.8%
Ion Exchange Column	17.1%	11.3%	11.3%
OPEX [M$/year]	**1.69**	**2.78**	**2.86**
UASB	41.2%	54.1%	54.2%
Electricity Generator	14.4%	16.4%	16.4%
Sand Filter	14.1%	9.4%	9.3%
Struvite Crystalizer	13.2%	8.8%	8.8%
Ion Exchange Column	17.1%	11.3%	11.3%
SALES [M$/year]	**2.57**	**4.19**	**4.25**
Electrical Power	80.4%	83.5%	83.5%
Struvite fertilizer	6.2%	4.0%	4.0%
Ammonia	13.4%	12.5%	12.5%
NPV [M$]	**−7.68**	**−10.75**	**−10.93**

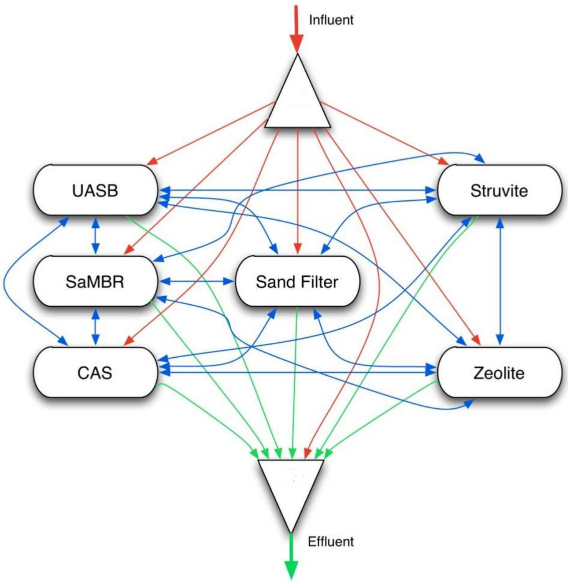

Figure 1: Illustration of a simple superstructure layout.

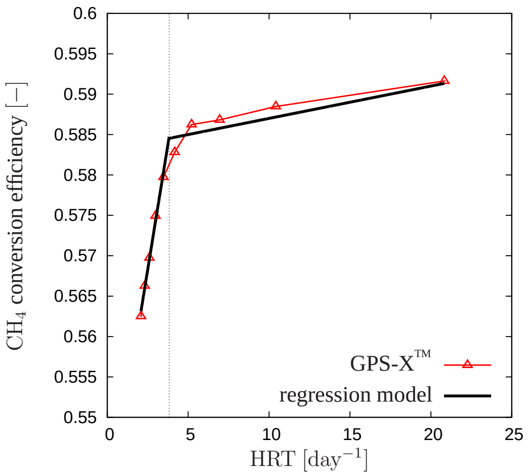

Figure 2: Illustration of a piecewise-linear performance model obtained from GPS-X™ simulated data.

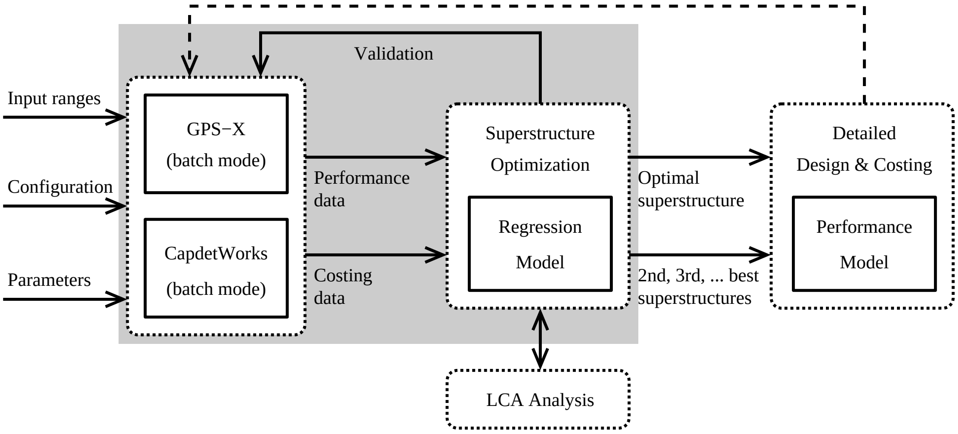

Figure 3: Illustration of the proposed methodology based on superstructure optimization and regression models.

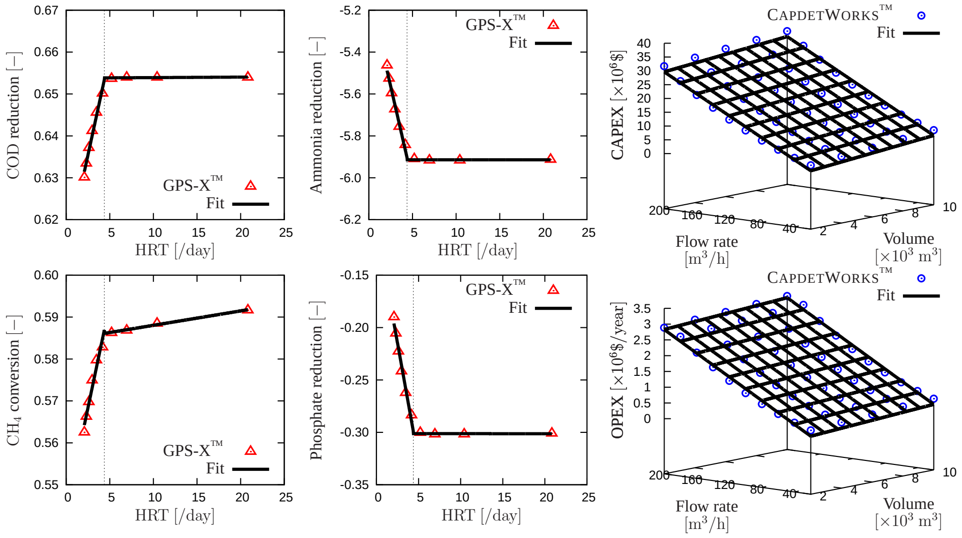

Figure 4: Subset of regression models for performance and cost prediction of a UASB unit. Top-left: COD reduction vs. HRT; Bottom-left: COD conversion into CH_4 (expressed as equivalent COD) vs. HRT; Top-center: Ammonia reduction vs. HRT;[a] Bottom-center: Phosphate reduction vs. HRT;[a] Top-right: CAPEX vs. unit volume and influent flow rate; Bottom-right: OPEX vs. unit volume and influent flow rate; Legend: Solid lines represent regression fits; Triangles denote GPS-X™ simulation results; Circles denote CAPDETWORKS™ simulation results.

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[a] Negative reduction ratios for ammonia and phosphates indicate a net increase due to the conversion of other forms of N and P inside the bioreactor.

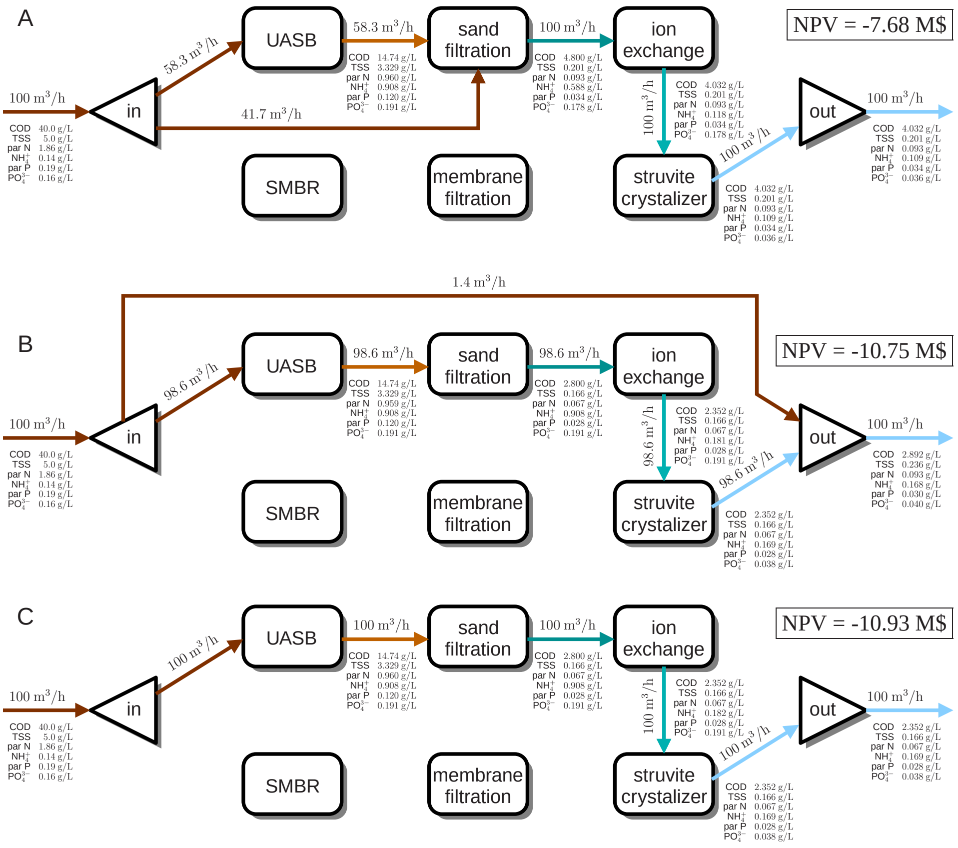

Figure 5: Optimal superstructures for the case study. A: No further restrictions on the interconnections; B: Bypass from source to sand filter not allowed; C: Bypass from source to sand filter or source to sink not allowed.