Decision support system for selecting the optimal WWTP configuration including resource recovery units

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Abstract

Purpose: The effort to upgrade urban WWTP into bio-refineries capable to recover and to produce valuable resources is hindered by the fact that technical, economic and environmental impact analyses are complex and time expensive. In the present work, we build a Decision Support System (DSS) that finds an optimal configuration of a WWTP given a set of resource recovery unit processes.
Methods: For the case study, we consider seven innovative technologies that are tested in the frame of the SMART-Plant H2020 project (No.690323). These technologies are modelled and integrated inside a plant-wide model superstructure with the aid of Modelica and Python programming languages.
Results: We present a novel framework for the design of WWTP under dynamic inflow conditions that depend on the local weather history, sewer characteristics and effluent limitations. The design is performed under a multi-criteria approach, where all the possible optimized WWTP-configurations given by the superstructure are sorted out based on economic, effluent quality and environmental impact criteria.
Conclusions: The developed DSS will be used to advise the potential stakeholders on how to implement the SMART-Plant Technologies for their specific wastewater treatment problem.

1. Introduction

In the last few decades, the wastewater treatment industry has experienced an outstanding rise in the variety of process technologies. Technology selection and benchmarking for plant retrofitting or new design have become more challenging than ever because of the large number of possible plant-designs for a given wastewater treatment problem. On top of this, politic initiatives that promote circular economy motivated the wastewater treatment sector to look for designs that could recover the most of resources from a wastewater stream while still meeting legislation limits. One of the reasons why new technologies for resource recovery are difficult to implement is that a benchmark analysis for a given case study is very complex. This is a key barrier to their exploitation since it increases the risk aversion of water utilities in moving from conventional technologies to techs with embedded additional benefits from recovery of resources.

DSS tools can help a decision maker to improve the operation of an existing plant ([10], [5], [23] and [24]) or help to choose an optimal plant design. In the last case, a knowledge-based DSS methodology is proposed by Comas [4] and Garrido-Baserba [8], where the main goal is to reduce the number of possible plant configurations to a reasonable sub-set of options. Once the sub-set is available, computationally expensive wastewater treatment process design and selection can be performed. Bozkurt [3] build a WWTP superstructure made of static process unit models, that use Mixed Integer (Non)linear Programming (MINLP) for optimal plant design. This approach has the advantage of relying on robust MINLP solvers and to have a relatively low computational complexity, but has the limitation that only steady-state process models can be used. Generally, resource recovery process models are described by complex dynamic models (i.e. ASM2d, ADM1 with P precipitation, etc.) with embedded control strategies: in this case a steady-state approximation could be extremely difficult to build. Moreover, because of the dynamic nature of the wastewater inflow, plant designs based on the steady-state assumption usually end up in an over-design since the control system is neglected [20] and hard constraints are imposed over the effluent legal limits.

The limitations of steady-state plant designs call for a closer analysis using dynamic plant-wide models. Superstructure design optimization studies with dynamic ASM/ADM-type models are very rare in the literature. Rigopoulos and Linke [22] build a superstructure based on the ASM1 model that finds an optimal activated sludge process design for a given constant inflow condition, while Guerrero [9] benchmarked five types of enhanced biological phosphorus removal (EBPR) configurations with design parameters selected from reference engineering guide-books. However, none of them included side-stream processes that are known to influence considerably the overall design of the plant. The well-known plant-wide model BSM2 recently updated by Solon [23] or the nutrient recovery model (NRM) library [25] could be used for building dynamic model superstructures. However, to the best of the authors' knowledge there was no attempt to use those plant-wide models for DSS.

The goal of this paper is to develop a modelling framework for systematically building dynamic plant-wide model configurations and perform benchmark analysis in order to help water utilities to reduce their risk aversion against new wastewater treatment process units. Since this paper is a first step toward a DSS that performs benchmarks between optimal designs of hybrid dynamic plant-wide models, we will focus here on the description of the DSS software architecture and the modelling of seven innovative resource recovery technologies that were tested during the SMART-Plant H2020 project (No.690323).

2. Material and methods

2.1. General framework

The problem addressed in this paper can be stated as follows: if we are given a set of wastewater treatment and resource recovery process units in order to treat a particular wastewater, what is the best WWTP plant configuration possible that minimizes the Net Present Value (NPV), the Effluent Quality Index (EQI), the Frequency of Effluent Violations (FEV) and the GreenHouse Gas emissions (GHG)? The objective is to obtain a fast and reliable answer. In order to get a fast one, almost all of the analysis steps should be automatized, while to get a reliable answer the most important dynamics and processes should be accounted for.

The DSS software architecture was implemented in Python and Modelica object-oriented programming languages. Modelica is employed to mathematically model the sewer-WWTP system since it is an equation-based language with a strong support for the simulation of hybrid differential-algebraic equations (DAE). The open-source modelling and simulation environment called OpenModelica (www.openmodelica.org) is used to build and run component-oriented models. In Modelica, a component model encapsulates equations into a reusable form, where an instance of the component can be used in place of the equations it contains. In this way, a system model is assembled from model components, typically by dragging, dropping and connecting component and other subsystem models schematically with the OpenModelica Editor tool. On the other hand, Python is used to build the DSS user interface, scrap data from web-sites and on-line databases, run regression and probabilistic models, setup the input for the sewer-WWTP model and post-processes the simulation results.

2.2. Models used

The overall process model of the DSS consists of two main components: the inflow model and the WWTP model. The first is made of two sub-models: the weather and sewer model, implemented in Python and Modelica, respectively. The WWTP-superstructure' stages comprise one or more treatment and/or resource recovery process unit models. The latest are innovative technologies that were tested into the SMART-Plant H2020 project (No.690323) to empower the concept of circular economy. The following novel technologies are modelled and integrated inside a plant-wide model superstructure:

- *Dynamic fine-screen and post-processing of cellulosic sludge* (ST1) is built on a series of solid/liquid separation units that affect the effluent particulate COD fractions (i.e. carbohydrate, protein, lipids and relative inerts) of the wastewater flow in relation to the inflow TSS concentration.
- *Polyurethane-based anaerobic digestion bio-filter* (ST2a) enables biogas recovery from a strong COD loaded wastewater inflow.
- *Short-Cut Enhanced Phosphorus and PHA Recovery (SCEPPHAR)* main-stream process (ST2b), consists of two SBR, one for heterotrophic bacterial growth and another for autotrophic nitrifiers growth, an interchange vessel and a chemical reactor for P-recovery as struvite. PHA-rich sludge is recovered from the anaerobic purge of the HET-SBR. The system is an evolution of the system described by Marcelino [16].
- *Tertiary hybrid ion exchange for N and P nutrients recovery* (ST3) includes units for micro-screen filtration for secondary effluent solids removal, ion exchange process for ammonia removal with MesoLite media, ion exchange process for P removal with hybrid ion exchange media (HAIX) media [19], regenerant storage tanks (NaCl and NaOH), regenerant rinse water tanks and nutrient recovery processes.
- *Short-Cut Enhanced Nutrient Abatement (SCENA) and ordinary digestion side-stream process* (ST4a) enables the integration of conventional biogas recovery with energy-efficient and compact nitrogen removal and P recovery [15].
- *SCENA and CAMBI-enhanced digestion side-stream process* (ST4b) treat half of the generated waste activated sludge (WAS) in a CAMBI^{TM} thermal hydrolysis system, while the thickened primary sludge is mixed with the hydrolysed WAS stream before digestion [27].
- *Side-stream SCEPPHAR side-stream process* (ST5) enables the integration of conventional biogas recovery from sewage sludge with the energy-efficient nitrogen removal from sludge reject water and the recovery of PHA and struvite [1].

To ease the task of modelling complex bio-process models, a Python auto-code generation routine enables to translate a model described in MS-Excel sheets to Modelica-code and to check the stoichiometric mass balance.

Anaerobic digestion modelling is based on the ADM1 model proposed by Batstone [2], modified here for co-digestion (primary sludge, waste activated sludge and cellulosic sludge), P release/precipitation [26] and solids retention. We will call this model as ADM1coP. The interface model between ASM2d+N_2O and ADM1coP is based on the work of Solon [23] and incorporates the modification for co-substrate flows and particulate COD fractionation. For activated sludge, the ASM2d+N_2O model [17] is modified to account for the temperature effect on the biomass kinetics and ammonia and nitrite inhibition of the ammonia oxidizing bacteria (AOB) and nitrite oxidizing bacteria (NOB).

The complex discrete control systems for ST2b, ST4a, ST4b and ST5 are built with the Modelica standard library called StateGraph which enables to model discrete event and reactive systems in a convenient way based on the Grafchart method [14].

The objective of the inflow model is to provide rough estimates on hourly basis of the volumetric flow rate and constituents load. Those time-series depend on WWTP geo-location. The novelty of our inflow model is that it uses a weather database for the European and Mediterranean region to build the dry and wet weather time-series and enables to include uncertainty in an intuitive way. We use a one hour time scale since our focus is on WWTP design and retrofitting and not on the evaluation of control strategies where a sub-hour scale is needed. The inflow to the WWTP accounts for dry and wet weather conditions. The first one is due to the contribution from the urban and industrial utilities, while the second is generated from atmospheric precipitations.

The urban wastewater discharge model assumes that the daily discharged waste water probability distribution function (PDF) for a given urban area is known. The dry weather time-series is made by multiplying the connected daily-PDF with a per capita flow-rate or constituent time-series. Per capita flow-rate and constituent loading for total COD, TN and TP are built. The loading for soluble COD, TKN, NH_4^+ and PO_4^{3-} are derived by applying relative fractions (e.g. PO_4^{3-}/TP).

The hourly wet weather data are built starting from daily weather gridded data that cover Europe and Mediterranean regions for a time period from 1950-01-01 to 2017-12-31, taken from the European Climate Assessment and Dataset (ECA&D) project [11]. For a given WWTP design location, the E-OBS daily dataset is linearly interpolated and disaggregated on an hourly time scale. For this purpose, we use the open-source Python library MEteoroLOgical [7].

Finally, dry and wet weather flow-rates and mass constituent discharges are inputs to a simple 1D sewer model that accounts for first-flush effect and groundwater infiltrations.

3. Results and discussion

The DSS' framework for a WWTP superstructure with resource recovery units is presented in **Figure 1**, and its procedural steps are described as follows.

Step1: Design problem set-up. The user provides the scope (i.e. WWTP retrofit or new design) and the general parameters (WWTP location, population equivalents, legal limits, wastewater characteristics, etc.).

Step2: Wastewater inflow generation. Python scraps from the web-databases the missing information. Once all the data from the user and the web are collected, the wet/dry weather and sewer models are executed in order to produce a dynamic wastewater inflow time-series with a one hour time step. This step is skipped if the user provides its own time-series.

Step3: Superstructure generation and simulation. Python builds a superstructure model of the WWTP from all given processes and resource recovery units. In our case, the superstructure is fixed to six stages connected between them to reassemble a general WWTP. Each stage represents a section inside a WWTP where the goal of operation is common (pre-treatment, main-stream activated sludge, effluent refinement, anaerobic sludge digestion and anaerobic supernatant treatment). For example**,** *Stage1* performs wastewater pre-treatment using a conventional primary settler or a dynamic fine-screen for cellulosic sludge recovery. A stage can be left empty, indicating no change for the flow just passing by. Thanks to Modelica' *redeclare* construct, stages are easily replaced in order to build all the possible plant configurations. The OpenModelica Compiler (OMC) translates Modelica-code to C-code which is compiled to a stand-alone executable file for each specific configuration. Note that this superstructure is different from a typical MINLP superstructure where the plant design configurations are achieved by discrete integer variables that switch on/off the connections/flows between stages or process units. The typical MINLP formulation would imply to compile once a very big superstructure dynamic model, where the majority of state variables are dummy variables. That would slow down the simulation time unnecessarily. In order to generate a code suitable for efficient execution, the OMC symbolically manipulates the equations to reduce the nonlinear system. Thus smaller systems of equations are potentially better handled during this OMC step then bigger (dummy) models. The proposed DSS superstructure compiles all the possible design configurations one-by-one, achieving a lower simulation time because no dummy states are created (i.e. smaller numerical Jacobian matrix of the DAE solver, lower data storage overhead, etc.) and better exploitation of the equation reduction routines. Moreover, independent plant configuration models allow for parallel computing of simulations. All the configurations are simulated with initial design parameters values (e.g. tank volumes, solid/liquid separation unit capacity, etc.) taken from reference handbooks and expert knowledge. During the following design parameter optimization (*Step6*), those values could be refined for each (promising) configuration.

Step4: Objective values estimation. From the Python environment, the executable file is run and simulation outputs are post-processed to compute the objective values relative to economic, effluent quality and environmental impact criteria. EQI and FEV are defined according to Flores-Alsina [6]. The costing analysis is performed within NPV [21]. OPEX accounts for aeration energy, pumping energy, mixing energy, heating energy, external carbon source, sludge disposal, chemical addition, human resources, insurance, licences and equipment replacement during the plant lifetime. The CAPEX estimation relative to common process units is taken from reference literature ([12], [18]) and corrected according to the Chemical Engineering Plant Cost Index (CEPCI) published by the Chemical Engineering magazine. Resources that are recovered from the wastewater stream are struvite, PHA-rich sludge and biogas. Those are cash-flow benefits that potentially lead to a positive NPV estimation. Environmental impact assessment is limited to the estimation of the GHG following the procedure described in Flores-Alsina [6] with the addition of greenhouse gases related to the construction of a particular WWTP configuration.

Step5: Design configuration sorting. Based on the user weights for NPV, EQI, FEV and GHG, all the configurations are sorted by the Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) which was introduced by Hwang and Yoon [13]. Note that this sorting depends not only on the weights provided by the user, but even on the optimality of the design given the (initial) values of the design parameters. The FEV is an especially relevant criterion, since it relates to the legal effluent limits that should be satisfied by the configuration design.

Step6: Design parameter optimization. This is a step that could be very expensive to perform. Design parameters are refined by minimizing the NPV and constraining the FEV and other process parameters (i.e. HRT, SOR, etc.). Because of the expensive objective function evaluation, the user could stop the optimization when a feasible solution that satisfies the constraints is found. The sorting outcome from *Step5* can be used to reduce the number of design configurations to optimize (e.g. priority to top-graded configurations with a satisfied FEV constraint).

Step7: Uncertainty analysis. The WWTP inflow generator produces a distribution of time-series that could be used as an uncertainty input for the optimized plant configurations. After simulation, TOPSIS is recomputed for each sample and sorting results are checked for robustness. The advantage of this step is that parallelization of computation is a trivial task.

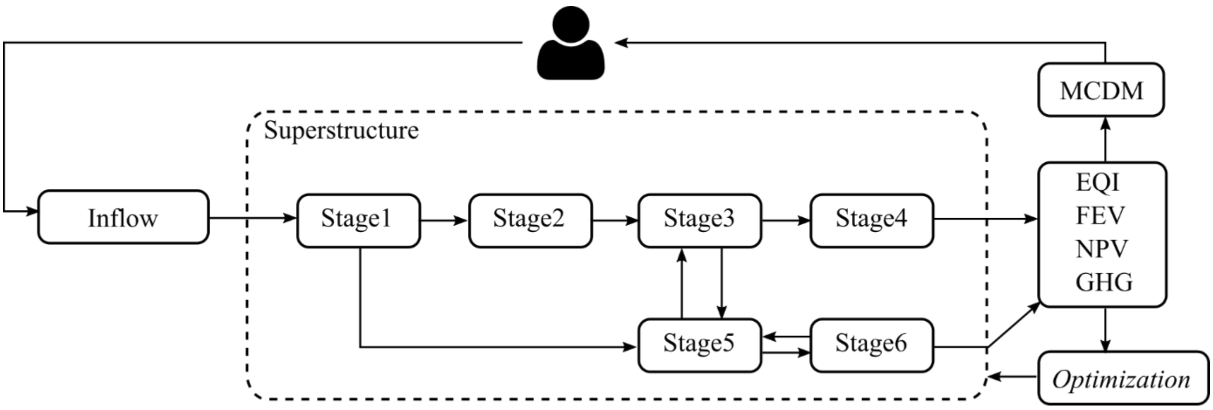

Figure 1. DSS framework for a WWTP superstructure with resource recovery units.

The case study that we present here is the design of a WWTP bio-refinery that can be assembled from SMART-Plant technologies (STs) and other conventional process units. **Table 1** lists the main process models available for each superstructure stage. An overall of 120 WWTP plant configurations are possible combining the conventional process units with the seven STs. To reduce this number, a process unit incompatibility matrix is used to find the uninteresting combinations. For example, ST3 in *Stage4* should not be preceded by A2O in *Stage3* since all the N and P would be removed: in this case, HRAS is the right "pre-treatment" design choice for ST3.

After all the relevant plan design configurations are available for simulation, the objective values are computed for each configuration (*Step4*) and if necessary design parameter optimization is performed within

Step6. Since the framework does not include an *ad-hoc* model calibration and validation step, absolute objective values have just a relative meaning. Because of this, the DSS performs the final sorting of the configurations by benchmarking all the ST-configurations against a base case represented by a conventional EBPR plant configuration (i.e. PS+A2O+AD). In other words, an objective value relative to a ST-configuration is subtracted against the base configuration to compute the benchmark objective values of EQI, FEV, NPV and GHG. Finally, those relative objective values are sorted by TOPSIS and the best configuration is available to the decision-maker.

Table 1 Process models available for each superstructure stage. SMART-Plant technologies (ST) as described in Section 2.2 and conventional process units such as rectangular primary settler (PS), modified Ludzack-Ettinger activated sludge process (A2O) and high rate activated sludge for COD removal process (HRAS), conventional anaerobic sludge digestion (AD) and anaerobic sludge digestion and fermentation (ADF).

	Empty	**PS**	**A2O**	**HRAS**	**AD**	**ADF**	**ST1**	**ST2a**	**ST2b**	**ST3**	**ST4a**	**ST4b**	**ST5**
Stage1													
Stage2													
Stage3													
Stage4													
Stage5													
Stage6													

4. Outlook

The framework of DSS based on Python and Modelica languages for the design of WWTP bio-refinery for resource recovery has been presented. There are several potential strengths that emerge from the developed framework: (i) only open-source software is used, which makes the DSS cheap and appealing for a future collaborative development; (ii) the full potential of Python' scientific libraries and Modelica' component-oriented modelling expands the range of benchmark analysis; (iii) the evaluation of the many plant configurations is flexible and easy to scale-up; and (iv) the geo-location of the plant design is accounted for. This last feature of the DSS is particularly important for the evaluation of the SMART-Plant Technologies since inflow characteristics and weather conditions could play an important role in the final sorting of the plant configurations.

In relation to the SMART-Plant project, the DSS will be used to advise the potential stakeholders on how to implement the SMART-Plant Technologies for their specific wastewater treatment problem. The purpose of the DSS is to lower the complexity of benchmarking resource recovery technologies, while still relying on the latest process knowledge available from the scientific community. Our framework includes the estimation of economic (i.e. NPV), effluent quality (i.e. EQI and FEV) and environmental impact (i.e. GHG) multi-criteria in order to set the decision making process in line with the holistic view of circular economy.

For future work, the DSS framework offers many development opportunities: (i) other resource recovery technologies could be integrated easily thanks to the component-oriented Modelica language; (ii) the inflow model range of application could be increased if connected with other weather databases like for example Daymet that covers North America; (iii) the environmental impact assessment could be further developed thanks to Python' Life Cycle Analysis frameworks (e.g. Brightway2 or openLCA); (iv) global optimization strategies should be tested for the design parameter optimization step in order to minimize the time of computation; and finally (v) a user friendly interface web-application should be built in order to simplify and standardize data input and results reporting.

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