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A process synthesis tool for WWTP – An application to design sustainable energy recovery facilities

Chitta Ranjan Behera, Resul Al, Krist V. Gernaey, Gürkan Sin*

Process and Systems Engineering Center (PROSYS), DTU Chemical Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

*Corresponding Author: Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, 2800 Kgs. Lyngby, Denmark, Email: gsi@kt.dtu.dk, Tel: +45 45252980

NOMENCLATURE

Symbol	Description
AD	Anaerobic digestion
CAPEX	Capital expenditure
DW	Dewatering
ERBF	Enhanced rotating belt filter
GHGs	Greenhouse gases
HRAS	High-rate activated sludge
HRT	Hydraulic retention time
IFAS	Integrated fixed-film activated sludge
LHS	Latin hypercube sampling
MC	Monte Carlo
MI(N)LP	Mixed integer nonlinear programming
MLE	Modified Ludzack-Ettinger
NER	Net energy recovery
NLR	Nitrogen loading rate
ODEs	Ordinary differential equations
OPEX	Operational expenditure
PC	Primary clarifier

PDEs	Partial differential equations
RBF	Rotating belt filter
SI	Supporting information
SOR	Surface overflow rate
SRT	Sludge retention time
TAC	Total annualized cost
TH	Thickener
Q_{in}	Influent flow rate
n	Plant life cycle
m_{CH_4}	Mass flow rate of methane (kg CH ₄ /d) gas
ϕ	Methane gas to the energy conversion factor
ψ	CO ₂ equivalent conversion factor
n_{RBF}	Number of RBF units
l	Plant layout
$\tilde{l}$	Set of top five plant layouts
f_i	Objective function
w_i	Weights for the objective function
V	Volume of reactor
g	Process constraint
y	Technology type
x	State variable
x_0	Initial condition of the state variable
u	Input
h	Process model
d	Design parameter
$\hat{d}$	Set of best design parameters of each layout
μ	Utility consumption
θ	Conversion efficiency
β	Kinetic parameter
γ	Stoichiometry coefficient

12

13 **ABSTRACT**

14 The objective of this paper is to present a new process synthesis tool to systematically synthesize, design,
15 and evaluate plant layouts for early-stage design/retrofit of wastewater treatment plants. The tool relies upon
16 an integrated methodology with the following key features: (1) first-principles mechanistic models used to
17 simulate existing and emerging technologies. This key innovation ensures predictive capability, 2) Monte
18 Carlo technique and simulation-based optimization techniques for handling the resulting computational
19 complexity effectively, 3) a systematic initialization algorithm developed for plant-wide simulation, 4)
20 optimizing design parameters, operational conditions, and plant layout simultaneously. Moreover,
21 stochastic analysis is performed to verify the robustness of plant configuration and design proposed by the
22 tool. Finally, using the tool, three real case studies are analyzed to demonstrate the design retrofit of WWTP
23 to the energy recovery plant.

24 **KEYWORDS**

25 Process synthesis tool, Simulation-based optimization, Process design, Stochastic analysis, Monte Carlo
26 simulation, Energy recovery

27 **RESEARCH HIGHLIGHTS**

- 28 • A novel tool to synthesize, design and optimize wastewater treatment plant layouts
- 29 • Handle multi-scale and multi-type process models
- 30 • A systematic initialization algorithm for dealing with plant-wide model simulations
- 31 • A holistic evaluation approach consisting of energy recovery, economic and sustainability
- 32 • The tool successfully applied to a retrofitting study of 3 full-scale plants

33

34

351. INTRODUCTION

36 In the 21st century, as we have started to acknowledge that wastewater is a renewable resource from which
37 water, energy, and materials can be recovered, the demand for building new resources recovery facilities
38 or retrofitting existing wastewater treatment plants (WWTPs) are gaining interest among various
39 stakeholders (such as utility managers, operators, regulators, end-users etc.). The primary problems in
40 deploying sustainable resource recovery technologies are lack of systematic planning and design
41 methodology, economic feasibility, market pull among others (Guest et al., 2009). Since the inception of
42 the activated sludge process, the horizon of innovative wastewater treatment solutions keeps on increasing
43 and so does the priorities. Several times the priorities set by the stakeholders are self-conflicting, which
44 further narrow the flexibility of decision-makers, for example, achieving stringent effluent quality and also
45 reducing the total cost of the project. Therefore competing objectives must be identified and trade-offs
46 made. Often design professionals are confronted with the fact that their proposed designs are not producing
47 desired results which may be due to unforeseeable social, economic, and legal changes (Dominguez and
48 Gujer, 2006). Moreover, some studies (Dominguez and Gujer, 2006; Vanrolleghem et al., 1996) advocate
49 that current design practices to build WWTP are not suitable to handle future developments as the
50 interaction among catchment area, sewer system, WWTP, regulatory body and public is hardly understood
51 and considered during the plant design stage. To handle the growing complexity, the decision-makers do
52 not have sufficient tools to carry out holistic analysis and are many times satisfied with the traditional
53 solutions based on heuristic approach (Balkema et al., 2002; Chamberlain et al., 2014; Guest et al., 2009).

54 Resource recovery from WWTPs in the form of energy (heat and/or electricity) has been a common
55 practice among developed nations, and the focus is now moving towards producing surplus energy from
56 an existing plant. For that matter a country like Denmark is leading to demonstrate the technical know-
57 how to build an energy recovery facility to other countries. Retrofitting existing plants or building new
58 recovery plants require a systematic understanding of COD diversion by adaptation of emerging
59 technologies such as Anammox technology and enhanced primary treatment technologies. Moreover, their
60 design and integration need to be optimized in order to maximize energy recovery and at the same time
61 respecting other constraints.

62 A process synthesis tool, which can also be called as decision support systems (DSS), has been
63 acknowledged as a realistic tool in the wastewater treatment field for various decision making process,
64 such as process synthesis, designing, control and monitoring (Bozkurt et al., 2015; Castillo et al., 2016b;
65 Comas et al., 2004; Hamouda et al., 2009; Poch et al., 2004; Shim et al., 2002). DSS is an information
66 system which integrates database, models, expert knowledge and user interface, and aims to provide an

insightful platform where decision-makers can analyze and compare various designs and layouts of wastewater treatment plant. The typical implementation time spend on building a new WWTP varies from 6 to 8 years and 13 - 18 % of the time (~ 1 year) is spend on facility planning and preliminary design of plant (WEF, 2018). During this phase, evaluating alternative technologies as well as plant layouts is one of the critical milestones. Therefore selecting a robust plant layout which can recover resources from wastewater and at the same time withstand the unforeseeable uncertainty (such as climate change, stringent laws, etc.) is a clear expectation from design engineers and decision-makers.

Several studies (as summarized in Table 1) have been carried out to address wastewater process synthesis and design by considering different objectives such as economic, operational, and environmental feasibility. Most of them solved the problem by applying expert knowledge or empirical models. Moreover, some studies (Alasino et al., 2007; Ferrer et al., 2008; Rivas et al., 2008; Vidal et al., 2002) have used rigorous mechanistic modelling to synthesize and design plant layouts but are limited by the number of technologies (considering present scenarios) used in those study. Since the wastewater treatment technology innovation and its availability in the market is rapidly growing, understanding and handling complexity involved in synthesizing plant layouts with diverse technologies (including both conventional and emerging) is a clear gap needed to be addressed. A study by Bozkurt et al. (2015 b) addressed the above mentioned challenges by including a considerable number of technologies for process synthesis but did not have the flexibility to evaluate the design of treatment units at different influent, operating and design parameter values (such as HRT, SRT, DO set point, etc.).

Furthermore, to ensure robustness (i.e., capability to handle unforeseen events) of selected plant layouts, uncertainty analysis is a useful technique which has not been rigorously incorporated in the design process by the other studies listed in Table 1. Additionally, none of the studies evaluate the plant-wide performance objectives in detail (using mechanistic models) while screening alternative technologies. In other words, how a selected plant layout or specific design parameters and operational conditions of a plant layout performs in terms of TN, COD removal in each stage (i.e., primary stage, secondary stage, sludge digestion stage, etc.) is not studied (numerically solved), which may provide additional insight to decision-makers (Flores-Alsina et al., 2012). The underlying reason that the earlier studies did not employ high-fidelity mechanistic models is primary because of computational limitations and/or initialization issues/challenges, which create a significant bottleneck to successfully evaluate/simulate different plant-wide layouts.

In this study we used a pragmatic approach such as Monte Carlo (MC) based simulation optimization, that offers a suitable strategy to find optimal design parameters and plant layout, unlike other conventional approaches such as MI(N)LP employed in earlier studies. Since it is decided to use multiscale models, so

the traditional optimization solver may break down due to the degree of nonlinearity and stiffness imposed by the mechanistic model. MC methods are a well-established statistical solution approach albeit so far used predominantly for performing global sensitivity and uncertainty analysis (Al et al., 2019b; Benedetti et al., 2008; Flores-Alsina et al., 2012; Sin et al., 2011). In this study, we employed the MC methods to facilitate exploration of design space (consist of design parameters like HRT and SRT; operational parameters like DO setpoint of each process) quickly and effectively compared to classical numerical optimization algorithms, which relies on the calculation of derivatives of the objective function. Compared to genetic algorithms (such as particle swarm optimization), on the other hand, MC methods require a fewer number of function evaluations.

This paper presents a new process synthesis tool (called as SPDLab) which rely upon a proposed integrated methodology to manage the complexity of the problem and find novel and optimal plant layouts along with preliminary designs of each unit. This tool aims to combine several new features: (1) first-principles mechanistic models to simulate various energy recovery-oriented technologies. This key innovation ensures predictive capability, 2) MC technique and simulation-based optimization techniques for handling effectively the resulting computational complexity, 3) a systematic initialization algorithm developed for plant-wide simulation, 4) optimizing design parameters, operational conditions, and plant layout simultaneously. To find an optimal solution, several realistic constraints are imposed, and multiple objectives are formulated and solved under both deterministic (i.e., no data uncertainty) and stochastic (i.e., data uncertainty) conditions. The purpose of the SPDLab tool development is to support the plant designers/decision-makers with providing comprehensive comparison reports on different plant layout alternatives. Moreover, the tool aims to be more user-friendly, where the end-users can reprioritize their objectives by continually learning from the outcomes. Finally, the proposed tool is applied on three real full scale wastewater influents to demonstrate its potential for the design retrofit of energy recovery plants.

122 *Table 1 Review of existing process synthesis tools and their functionalities. The symbol tic (✓) means feature is present and cross (✗) means feature is absent.*

References	Objectives			Model fidelity		Technology types	
	Process synthesis	Process design	Performance evaluation ¹	Empirical	Rigorous mechanistic	Conventional	Emerging ²
(Tang et al., 1997)	✓	✗	✗	✓	✗	✓	✗
(Vidal et al., 2002)	✓	✗	✓	✓	✓	✓	✗
(Poch et al., 2004)	✓	✗	✗	✓	✗	✓	✗
(Alasino et al., 2007)	✓	✓	✗	✗	✓	✓	✗
(Zeng et al., 2007)	✓	✗	✗	✓	✗	✓	✗
(Rivas et al., 2008)	✗	✓	✗	✗	✓	✓	✗
(Ferrer et al., 2008)	✓	✓	✓	✗	✓	✓	✗
(Chamberlain et al., 2014)	✓	✗	✗	✓	✗	✓	✗
(Bozkurt et al., 2015)	✓	✓	✗	✓	✗	✓	✓
(Puchongkawarin et al., 2015)	✓	✗	✗	✓	✗	✓	✗
(Rawal and Duggal, 2016)	✓	✗	✗	✓	✗	✓	✗
(Garrido-Baserba et al., 2016)	✓	✗	✗	✓	✗	✓	✓
(Castillo et al., 2016b, 2016a)	✓	✓	✗	✓	✗	✓	✓
This Study	✓	✓	✓	✓	✓	✓	✓

123

¹ Performance evaluation objective aims to examine unit wise performance (with sufficiently detailed model) of plant layouts (contains multiple treatment technologies)

² Emerging technology types are Anammox, rotating belt filter, A-stage etc.

1242. **METHODS**

125 An MC based simulation-optimization framework was developed and evaluated successfully for various
 126 chemical engineering related case studies, such as working fluid selection, molecular process, and product
 127 design (Frutiger et al., 2019, 2016). The framework was further modified and adapted (as shown in Figure 1)
 128 in the context of wastewater treatment plant design. The integrated methodology has six steps which are
 129 explained in detail in the following sections. A graphical user interface of the process synthesis (SPDLab) tool
 130 is developed and presented in Figure S3 (see SI).

131

132 *Figure 1 Schematic representation of a systematic, integrated methodology used for the development of process synthesis tool shows*
 133 *the steps involved, implementation platform and the outputs from each step.*

134

132.1. Step 1: Define objectives

136 The first and foremost task of a process synthesis tool is to define the objectives. Based on that, the relevant
137 key performance indicators (KPIs) and constraints are framed into a single or multi-objective optimization
138 problem. Users/decision-makers identify whether to retrofit or newly design a plant for a given influent
139 wastewater. Generally, several objectives such as minimizing the total annualized cost (TAC), maximizing net
140 energy recovery (NER), minimizing greenhouse gas emissions (GHGs) are considered as KPIs. Moreover,
141 other aspects, namely complying with stringent effluent discharge limits, operational flexibility, etc. can also
142 be imposed as constraints. Often the relative importance of objectives may not be evident or cannot be
143 generalized due to several factors, such as geopolitical, economic, market, etc. Therefore, finalizing the
144 objectives, which are critical to the solution of the problem, is an iterative process which needs consultation of
145 experts and rigorous investigation of several considerations (as explained above). The outcome of this step can
146 be a decision aiming at retrofitting a specific unit of the existing plant, or extending the capacity of the existing
147 plant, or designing a completely new plant.

142.2. Step 2: Data acquisition, process model library development, and customization

149 In the second step, various types of data, such as influent wastewater load (flow, COD, TN etc.), design and
150 operational parameters (HRT, SRT, SOR etc.), utilities and equipment cost (electricity price, chemical cost
151 etc.), space availability (of different WWTP plant site) are collected from design handbooks (Metcalf and
152 Eddy, 2003; WEF, 2018), previous studies (Bozkurt et al., 2016; Lackner et al., 2014; Malovanyy et al., 2015b;
153 Vázquez-Padín et al., 2014), commercial databases (CapdetWorks 4.0), and personal communication with
154 plant managers. These data are further passed through a sanity check to ensure data consistency (using process
155 understanding), and then stored in Excel for executing the subsequent steps. Based on the selected objectives
156 (i.e. in Step1), promising technologies (combination of conventional and emerging) are selected by using the
157 process knowledge gathered from the literature (Batstone et al., 2002; Behera et al., 2018; Gernaey et al., 2014;
158 Lotti et al., 2014; Malovanyy et al., 2015a; Metcalf and Eddy, 2003; Smitshuijzen et al., 2016; Vázquez-Padín
159 et al., 2014; WEF, 2018). For example, the primary treatment units, such as primary clarifier (PC), rotating
160 belt filter (RBF), enhanced rotating belt filter (ERBF) and high rate activated sludge (HRAS), can be
161 considered as potential primary treatment alternative technologies for meeting higher energy production
162 objectives. Likewise for the mainstream, energy-efficient technologies, such as Anammox with different
163 carrier size (granular type named ELANM; AnoxKaldnes K₁ carrier-based named IFAS) and conventional
164 activated sludge (MLE type), can be considered. Moreover, anaerobic digestion (AD) and sidestream
165 Anammox (granular type named ELANS) can be considered to boost net energy production in the plant to be
166 designed. Each technology in the customized library can be modeled using a hybrid approach (i.e., empirical
167 as well as mechanistic models) depending on the purpose or level of detail required, for example, if it is

168 intended to compare the performance unit by unit of alternative plant layouts, then higher fidelity models (such
169 as ADM1, ASMG1, 1-D biofilm, etc.) should be considered to model each technology. Moreover the model
170 library is flexible and can be customised such that users can add or remove a technology from the model library.
171 It is essential to highlight here that the complexity of the selected model needs to be considered to explain the
172 phenomena in a process unit in a sufficiently detailed manner. The configuration and modelling approach for
173 a customized technology library is presented in Table 2.
174

Process Configuration	Modelling approach
<p>The conventional activated sludge system is modeled as a Modified Ludzack-Ettinger (MLE) process (inspired from the study (Gernaey et al., 2014)) where anoxic tanks (for pre-denitrification and COD reduction) are followed by oxic tanks (for nitrification and COD reduction). There is also a provision to add external carbon in anoxic tanks for enhancing denitrification. The ASMG1 (Guo and Vanrolleghem, 2014) is used to model both anoxic and oxic tanks whereas the secondary clarifier (SC) is modeled as a non-reactive settler using an exponential settling velocity function (Takács et al., 1991).</p>
<p>To model carrier-based mainstream Anammox process, an integrated fixed-film activated sludge (IFAS) configuration is selected (motivated from the successful pilot-scale study by Malovanyy et al., (2015a). A multiscale modelling approach is implemented where the biomass growth in carriers (i.e., Kaldnes K_1 type) are modeled as one dimensional (also used in other studies (Eberl et al., 2006; Lindblom et al., 2016). The reactor is assumed as a completely stirred tank reactor (CSTR), and diffusion governs the transport of soluble compounds, whereas the particulates are transported by advective transport. Validation of the IFAS model is presented in the supporting information section 6 (SI.6). The SC model is the same as in the case for MLE (see above explanation).</p>
<p>For both mainstream and sidestream granule based Anammox, a one dimensional (assuming spherical geometry) biofilm growth approach (as explained in Vangsgaard et al., (2013) is adopted. For plant-wide simulation, the reactor is implemented as a CSTR type by maintaining the same SRT as in the original SBR. Validation of the granule model is presented in SI.7.</p>

<p>The PC is modeled (as explained in Gernaey et al., (2014) and Otterpohl et al., (1994) by assuming it as a continuous stirred tank where effluent of the tank is separated in to primary clarifier effluent and sludge.</p>
<p>The anaerobic digester (AD) is assumed to be a CSTR type where a mixture of primary settled sludge and biomass produced in the mainstream are digested to produce biogas and modeled using the Anaerobic Digestion Model no 1 (ADM1) (Batstone et al., 2002).</p>
<p>Both the RBF and ERBF units work based on cake filtration and sieving and are model using a hybrid approach, i.e., combined empirical and dynamic model discussed in other studies (Behera et al., 2018; Boiocchi et al., 2019). For ERBF, the polymer effect on carbon removal is also captured in the model. The particulate COD (X_S), inert particulate COD (X_I), biomass (X_{BH}) have different efficiencies and are correlated with TSS removal efficiency. Additional explanations of the RBF and ERBF models are provided in SI.8.</p>
<p>The HRAS is modeled as a conventional activated sludge system, but the HRT and SRT are kept relatively low (see Table S3, in SI) to avoid COD oxidation and nitrification. A simplified validated model presented in the study by Smitshuijzen et al., (2016) is used here. Moreover, the settler is modelled as an ideal separator (similar to PC as discussed above), and the particulate removal efficiency is considered to be 98.5% (Smitshuijzen et al., 2016).</p>
<p>The thickener and dewatering are modeled by applying a constant TSS removal efficiency (98%) and f_{thick} and f_{dewat} factors (as explained in the study by Gernaey et al., (2014)) to separate sludge and effluent water.</p>

172.3. Step 3: Design parameter selection, sampling and dimensioning of technology

178 *Design space exploration using Monte-Carlo procedure*

179 At this stage, the total number of technologies that need to be evaluated is finalized. So to design each
180 technology, relevant design parameters and their suitable range, which is also called the design space, need to
181 be selected. Widely used design parameters are HRT, SRT, SOR, NLR, recycle ratio, volume ratio, etc. whose
182 value can be taken from the database developed in the previous step. It is important to note that the critical
183 design parameters of emerging technology (effectively the scale-up criteria) need to be cross-checked and
184 ideally validated by technology developers. Along with design parameters, some essential/critical operation
185 parameters can be considered while designing an individual unit. For example, when the objective is to harness
186 surplus energy from WWTP, it is not appropriate to maintain a very high DO set point for the aerobic processes,
187 which can add unnecessary energy consumption. Besides, for some processes like Anammox, a high DO
188 setpoint does not help to maintain the stability of the process (Agrawal et al., 2018; Cao et al., 2017; Lauren
189 et al., 2016; Vázquez-Padín et al., 2014; Zhou et al., 2011).

190 MC methods are a well-established statistical sampling technique. The basic principle is to characterize the
191 input parameters; here it is design parameters by a probability distribution function such as normal, uniform
192 or Gaussian-based on the degree of belief concerning where the appropriate values of the parameter will lie
193 (Al et al., 2019b; Sin et al., 2009). For a plant layout, different parameter sets of each unit (such as primary,
194 secondary, etc.) can be combined and sampled using the Latin hypercube sampling (LHS) technique. In this
195 way, the impact of more than one change of a parameter (i.e., the simultaneous variation of design parameters)
196 at a time is captured. Furthermore, it gives a free hand to evaluate all the design parameters to be considered
197 and select the best one for a given objective.

198 *Dimensioning of technology*

199 Each technology's basic design, such as area, volume, height, etc. needs to be calculated for a given wastewater
200 design challenge (i.e., capacity and wastewater composition). The outcome of this is two-fold: Firstly, it will
201 give an idea about the space requirement, and second this information is needed for the subsequent plant-wide
202 simulation to calculate the performance. Therefore each technology can be designed using the following design
203 procedure.

204 *Dimensioning of primary treatment alternatives*

205 For the primary clarifier the surface area and the volume of the tank can be calculated by using the Equations
206 1 and 2.

$$A_{PC} = \frac{Q_{in}}{SOR} \quad 1$$

$$V_{PC} = A_{PC} \times height \quad 2$$

Likewise, for the RBF and ERBF, a typical Salsness filter (SF2000) model design is adopted. So the number of RBF units and the total volume required for a given wastewater flow rate is calculated by Equations 3 and 4.

$$V_{RBF} = n_{RBF} \times V_{SF\ 2000} \quad 3$$

$$n_{RBF} = \frac{Q_{in}}{Q_{avg, SF\ 2000}} \quad 4$$

The HRAS unit contains an aeration tank for carrying out biosorption, and a clarifier to separate the suspended solids. So, the volume of the HRAS unit (including both aeration tank and settler) can be calculated using Equation 5.

$$V_{HRAS} = HRT_{HRAS} \times Q_{in} + 0.023 \times Q_{in} \quad 5$$

Dimensioning of secondary treatment alternatives

Relevant secondary treatment technologies are MLE, ELANM, and IFAS. To design MLE, a conventional approach is used. The MLE has three sections: pre-denitrification (anoxic tank), nitrification and COD oxidation (aerobic tank) and a settler.

The volume of the aerobic tank can be calculated by Equation 6 and of the anoxic tank by Equation 7. The total volume of the MLE can be calculated by Equation 8.

$$V_{aerobic} = HRT_{aerobic} \times Q_{in, MLE} \quad 6$$

$$V_{anoxic} = V_{aerobic} \times VR_{MLE} \quad 7$$

$$V_{MLE} = V_{anoxic} + V_{aerobic} \quad 8$$

The volume of ELANM which operates in SBR mode can be calculated based on nitrogen loading rate (NLR), which is given by Equation 9. For mainstream, the flow rate is quite high, so multiple ELANM tanks should be considered and place either in parallel or stackwise based on the space availability and civil engineering advancement, which depends on local conditions.

$$V_{T, ELANM} = \frac{TN\ load}{NLR} \quad 9$$

For the IFAS, it has two sections, i.e., an aeration section and a clarifier section and it operates in continuous mode. The volume of the aeration tank can be calculated by Equation 10 and of the clarifier by Equations 1

235 and 2. The total volume of the IFAS can be calculated by summing up aerobic tank volume and clarifier
236 volume.

$$237 \quad V_{aerobic, IFAS} = \frac{TN \text{ load}}{NLR} \quad 10$$

238

239 *Dimensioning of sludge stabilization alternatives*

240 For treating the sludge, AD is used which is assumed to operate in CSTR mode (and also in mesophilic
241 condition) without any recycle. So the HRT and SRT are the same for the AD. The volume of the AD can be
242 calculated based on Equation 11.

$$243 \quad V_{AD} = SRT_{AD} \times Q_{in, AD} \quad 11$$

244 *Dimensioning of sidestream treatment alternatives*

245 The sidestream wastewater, which is also known as reject water from sludge treatment, is rich in TN load and
246 the flow rate quite low compared to the mainstream. Here ELANS can be considered, and its volume can be
247 calculated by using ELANM approach (i.e., Equation 9).

248

249 **2.4. Step 4: Plant layout generation, initialization, and simulation**

250 ***Superstructure formation***

251 In this step, using all the selected technologies (in step 2) a superstructure is formed (as shown in Figure 4),
252 which consists of different wastewater sources, treatment layers (such as primary, secondary, sludge treatment,
253 etc.) and sinks. The superstructure can be formulated in three different ways, such as alternative collection,
254 combinatorial synthesis, and insight-based synthesis. The *alternative collection* method uses all the known
255 WWTP layouts based on previous experiences, literature, etc. to form the superstructure. This method heavily
256 depends on experience and does not allow us to evaluate emerging technologies. However, the combinatorial
257 approach generates a superstructure which combines all possible integration of technologies, resulting in vast
258 search space. Many times the superstructure contains redundant and unrealistic plant layouts (for example
259 treating wastewater by bypassing treatment technologies to sink) and increases the required computational
260 effort unnecessarily. The last approach, which is called *insight-based*, eliminates unfeasible and non-
261 convenient alternatives based on process knowledge and addresses the shortcomings of the above two methods.
262 The insight-based approach has been used for wastewater process synthesis (Al et al., 2019a; Bozkurt et al.,
263 2015; Castillo et al., 2016a; Quaglia, 2013) and is also adopted for this study.

264 **Initialization of plant layout and simulation**

265 Since the methodology uses computational demanding consensus models (such as ADM1, 1D Biofilm, etc.),
266 which can be based on ODEs, PDEs or a combination of both, a common problem encountered during
267 simulation is improper initialization. That is assigning a suitable starting point for the simulation. Moreover,
268 the situation gets worse in a plant-wide simulation where multiple units are connected and recycles are present.
269 Before simulating the plant layout, proper initialization of each unit is required to avoid convergence issues
270 due to the presence of non-linearities and stiffness in the model equations. The initialization is a long-standing
271 issue which is typically solved by a trial and error approach (Gernaey et al., 2014; Pons et al., 1999). Therefore,
272 a systematic initialization strategy is necessarily anticipating the model complexity and the interactions
273 between unit process models during simulations. Furthermore, the proposed design methodology is heavily
274 dependent on plant-wide simulation for optimizing plant layout and design. To handle the initialization issues,
275 a sequential approach is used here. That means once a plant layout is generated from the superstructure, it
276 passes through several steps (as shown in Figure 2) sequentially based on the complexity of the network (i.e.,
277 presence of recycle, without recycle, etc.) to find suitable initial conditions for the entire plant. An example
278 based on the steps presented in Figure 2 is illustrated in SI section 5.

279 At this stage, plant layouts, models of each unit, and initial conditions are finalized. So now, steady-state
280 simulations can be performed using the selected influent wastewater. A solver like *ode15s* (recommended for
281 stiff problems) can be used in the MATLAB Simulink environment to simulate the plant-wide model. All the
282 plant layouts can be simulated several times (i.e., for each LHS sample as discussed in earlier steps), and data
283 on KPIs (such as NER, GHGs, TAC, etc.) can be calculated and stored for the next step analysis. Parallel
284 computing features of MATLAB should be exploited to manage the computational demand and reduce
285 simulation time, i.e. several plant layouts can be simulated simultaneously.

286

Figure 2 Illustration of sequential approach to initialize a plant layout. Firstly, the plant layout is divided into multiple sub-layouts, and each sub-layout is initialized and simulated to find appropriate initial conditions for the plant layout. Here V is the volume of the reactor and x is the state variable which needs an initial point.

2.5. Step 5: Deterministic plant layout and its design selection

To find the best plant layout and its optimal design parameters under deterministic conditions (i.e., not accounting uncertainty), a two-tier approach can be considered. Firstly, the optimal design parameter set for each plant layout needs to be determined. Then, among the plant layouts, the top five plant layout, candidates should be selected for stochastic analysis. Consequently, it can be treated as bi-level optimization. Therefore, a typical multi-optimization problem can be represented by Equations 12 to 15.

$$\text{maximise } f_1 := \text{NER (kWh/d)}$$

$$\text{minimise } f_2 := \text{GHGs (kg CO}_2 \text{ / d)}$$

$$\text{minimise } f_3 := \text{TAC (Euro / m}^3 \cdot \text{yr)}$$

12

Subject to;

Process model

$$h(u, x, \theta, \gamma, \beta, \mu, d) = 0$$

13

Process constraint

$$g(x, y) \leq 0$$

14

Structure constraints

$$x^{LB} \leq x \leq x^{UB}$$

$$x \in R^n, y \in \{0;1\}^m$$

15

where f is the objective function, x is the continuous variable representing design and operational variables (e.g., HRT, SRT, etc.) defined by their upper (x^{UB}) and lower bound (x^{LB}) in a continuous feasible region R

309 , y is a binary variable representing alternative technology (e.g., PC, RBF, etc.), g and h are process models
 310 (e.g., ADM1) and process constraints (e.g., effluent COD, TN, etc.). $u, \theta, \gamma, \beta, \mu, d$ are the input, conversion
 311 efficiency, stoichiometry coefficients, kinetic parameters, utility consumption, and design parameters,
 312 respectively.

313 **Selecting an optimal design parameter set**

314 To choose the best design parameter set for each plant layout, the optimization problem, as proposed above,
 315 can be solved by a weighted scoring method, as presented in Equation 16. Before that, each objective function
 316 value is normalized to eliminate the influence of its magnitude on the solution. The value of each weight ($w_1, w_2, w_3 \dots w_n$)
 317 can be decided based on the priorities set by the end-user. For example, if all the three
 318 objectives are equally important, then $w_1 = w_2 = w_3 = 0.33$ should be used. This approach is also used in other
 319 applications (Flores-Alsina et al., 2008) and flexible enough to provide solutions when the end-users priority
 320 changes or he/she is not sure and want to decide by learning from observations. So finally, the optimal/best
 321 design parameter set can be selected by sorting the score (i.e., J) and picking the maximum or minimum based
 322 on the objective. For example, the energy recovery objective should be maximized, whereas total cost and
 323 greenhouse gas emission should be minimized. So when a mixture of self-conflicting objectives are present,
 324 then a positive sign should be used for maximization objective functions and negative sign should be used for
 325 minimization objective functions to calculate a net score (J).

$$326 \quad J = w_1 \cdot f_1 + w_2 \cdot f_2 + \dots + w_n \cdot f_n = \sum_{i=1}^n w_i \cdot f_i \quad 16$$

327 **Ranking top five layouts**

328 Once the design parameters of each plant layout are finalized based on the above procedure, the next task is to
 329 rank all the feasible plant layouts and pick the top five layouts for stochastic analysis. The number five is an
 330 arbitrary choice, but this number can be reduced or increased based on the computational facility that is
 331 available. The ranking of the plant layouts can be done by using a weighted scoring approach similar to the
 332 method used for selecting optimal design parameters.

332.6. Step 6: Stochastic analysis of selected plant layouts and respective designs

334 Stochastic analysis is performed to verify the robustness of the deterministic solutions (i.e., the outcome of
 335 step 5). This is an essential step from a wastewater treatment process synthesis and design point of view
 336 because a higher uncertainty in the influent pollutant load (not accounted for during design) arriving at the

337 plant can offset the plant performance. The conventional approach used by the design engineer to tackle the
338 uncertainty is by using a safety factor. So, in that approach all the uncertainty sources are lumped to the safety
339 factor, which often leads to an overly conservative design (Belia et al., 2009). To avoid this, an evaluation of
340 all the deterministic solutions needs to be performed under uncertainty. It can be done systematically by
341 following the steps explained below.

342 ***Define input uncertainty and perform a plant-wide evaluation***

343 To define input uncertainty, expert knowledge is used. From a wastewater point of view, the influent
344 wastewater data are highly uncertain because of variation in sources of generation (such as domestic and
345 industrial) and due to climate change over the years. More specifically, the flow rate, the temperature, the COD
346 fractions, and the nitrogen fractions in wastewater change over time (daily, weekly, seasonal) and these
347 variations need to be considered while designing a plant. Likewise, temperature variation (affecting the activity
348 of bacteria), cost data (utility cost, tax, etc.), equipment performance over time, etc. can be other sources of
349 uncertainty to consider during the design/retrofit stage. Some studies (Al et al., 2019b; Sin et al., 2009)
350 highlight that influent load is more influential to the performance of the wastewater treatment plant. However,
351 the selection of uncertainty is very subjective and depends on the end users priority and expert knowledge.

352 Once the uncertain parameters are identified, a probability density function (such as normal, uniform,
353 Gaussian, etc.) is assigned based on experimental data/prior knowledge or assumptions for the distribution of
354 individual parameters. Each distribution is described by its mean, minimum, and maximum values, which are
355 later used for MC simulations. The LHS technique by Iman and Conover (1982) is used to generate a fixed
356 number of samples, which also takes into account the correlation among input parameters.

357 The selected plant layouts from the deterministic step (i.e., 5) are simulated several times using the uncertain
358 input samples generated in the previous step by LHS. The outcome is a distribution for each output, for
359 example, the net energy production, total annualized cost, greenhouse gas emission, etc. This analysis further
360 helps to understand the influence of input uncertainty on the KPIs/objectives of the treatment plant to be
361 designed.

362 ***Decision making under uncertainty***

363 Using the simulated data generated in plant-wide simulation and simple statistics, such as mean and percentile
364 calculation, the 95% confidence interval can be calculated for selected KPIs. Along with that, for each plant
365 layout the effluent violation in % should be calculated to highlight the robustness of the deterministic solutions
366 under uncertain scenarios. The plant layout that violates the effluent discharge limit several times (for example
367 more than 20%) can be eliminated. Then a ranking approach can be used to find the best and most resilient

368 plant layout by sorting the objective scores for the remaining layouts (after imposing effluent violation
369 constraints). For a multi-objective problem, the objective score can be calculated by a weighted sum approach
370 as already explained in step 5 (used for the deterministic approach). It is crucial to highlight that for each
371 objective function, mean values (calculated from simulation data) are considered, unlike the single value
372 approach in the deterministic step 5. Based on the priority, the objective scores are either to be minimized or
373 maximized.

374

375 **3. CASE STUDIES**

376 **3.1. The plant configuration**

377 To demonstrate the application of the process synthesis tool, two Danish WWTPs (Avedøre and Lynetten) and
378 one Spanish WWTP (Valladolid) were analyzed. The Avedøre WWTP, located in the west of Copenhagen,
379 can treat 750,000 PE wastewater. The Lynetten WWTP is located in the east of Copenhagen with the capacity
380 to serve 265,000 PE. On the other hand, the Valladolid WWTP, situated in the northwest of Spain, has the
381 largest capacity compared to the Danish WWTPs, with approximately 1,067,000 PE. All the three treatment
382 plants have similar treatment units, such as primary treatment, biological treatment, sludge digestion, etc. (plant
383 layout is shown in Figure 3). The treated wastewater effluents of all three WWTPs are discharged to a
384 receiving water body whereas the produced sludge of the Danish WWTPs is further incinerated in a fluidized
385 bed incineration plant and for the Spanish WWTP it is used for agricultural applications. The current practice
386 is the recovery of energy from the biogas generated in the AD unit as heat and electricity. Both the Avedøre
387 and the Valladolid WWTP use a combined heat and power (CHP) engine to convert biogas to heat and
388 electricity, whereas Lynetten only produces heat using a boiler. The influent wastewater, which enters the three
389 plants, mainly contains organic pollutants, nutrients, suspended solids, etc. For this study, the removal of
390 pollutants, such as COD and TN, is given more importance as their concentrations are higher compared to the
391 other pollutants, and they are omnipresent irrespective of geographical boundaries. Secondly, the process
392 synthesis and design problem is addressed in a step by step manner. For each plant, the yearly influent loads
393 are presented in Table S12 (see SI).

Figure 3 Generic plant layout for the Avedøre, Lynetten, and Valladolid wastewater treatment plants.

3.2. Retrofitting scenarios: Objective function formulation

The primary objective is to assess the feasibility of designing energy recovery plants by modifying existing WWTPs, which will be analyzed in two different ways:

1. Maximize net energy recovery challenge: Synthesizing new plant designs based on proper selection and combination of primary, secondary, sludge digestion and reject water treatment units by prioritizing the net energy recovery objective only.
2. Sustainable, economic, and energy-efficient design challenge: Screening diverse treatment units and their combinations by considering sustainability and economic factors in addition to objective 1 (i.e., energy recovery) simultaneously. The cost primarily covers capital and operating expenses (such as electricity, chemical additions, etc.) and sustainability considers emission of GHGs from WWTPs.

The end use of effluent water is to discharge it to the water body. So a stringent effluent quality (i.e., COD < 100 g COD/m³, TN < 10 g N/m³ and NH₄⁺ < 1 g N/m³) constraints are imposed while finding the optimal solution. The problem is framed as an optimization problem, as shown in Table S13 (see SI).

3.3. Data acquisition, technology selection, and superstructure formulation

Since the methodology uses computational demanding consensus models such as the ASMG1, for process synthesis and design of biological units, it is apparent that the COD and TN concentrations present in the influent wastewater need to be characterized in more detail. For the COD fractionation, the crucial components are inert soluble compounds (S_I), inert particulates (X_I), readily biodegradable soluble compounds (S_S) and biodegradable particulates (X_S). For practical purposes, the influent biomass (X_{BH}, X_{AOB}, X_{NOB}, X_{AnAOB}, X_P) is assumed to be zero. Similarly, the soluble nitrogen component (S_{NO3}, S_{NO2}, S_{NO}, S_{N2O}, S_{N2}) and dissolved oxygen (S_O) in influent wastewater is also considered to be zero for all three plants. For the Avedøre and Lynetten WWTPs, the COD and TN are fractionated (as shown in Table 3) by applying a procedure explained elsewhere (Bozkurt et al., 2016).

422

423 *Table 3 Influent wastewater loads for the Avedøre, Lynetten, and Valladolid wastewater treatment plants. Components having zero*
 424 *concentration are excluded from the table.*

Parameters	Avedøre ³ (Bozkurt et al., 2016)	Lynetten ³ (Bozkurt et al., 2016)	Valladolid ⁴	Units
Capacity	265,000	750,000	1,067,033	PE
Q	72,000	162,465	213,408	m ³ /d
S _I	23.48	56.52	21.00	g COD/m ³
S _S	107.85	153.25	205.00	g COD/m ³
X _I	93.22	89.98	15.00	g COD/m ³
X _S	251.65	357.59	122.00	g COD/m ³
S _{NH}	32.85	45.60	19.40	g N/m ³
S _{ND}	0.00	0.00	4.94	g N/m ³
X _{ND}	9.80	5.40	7.42	g N/m ³

425

426 For the Valladolid influent wastewater, effluent measurements, such as total COD (TCOD_{eff}), particulate
 427 COD (pCOD_{eff}), total nitrogen (TN) and ammonium (NH₄⁺), are collected (see SI.9 for details). While
 428 fractionating the COD, it was assumed that the inert soluble COD remains constant (Bozkurt et al., 2016;
 429 Roeleveld and van Loosdrecht, 2002). That means that S_I in the influent is equal to sCOD_{eff}. Then, by
 430 subtracting the S_I from the influent soluble COD, the S_S concentration is calculated. Furthermore, it is also
 431 assumed that the influent X_I is equal to pCOD_{eff} by neglecting the contribution of dead biomass (X_P) to
 432 particulate effluent COD. The biodegradable particulate COD (X_S) is calculated by using the correlation
 433 X_S=TCOD - (S_S+S_I+X_I). For the organic nitrogen fractions, such as soluble organic nitrogen (S_{ND}) and
 434 particulate organic nitrogen (X_{ND}), these are calculated by assuming 40 % and 60 % of the organic nitrogen
 435 (which is the difference between TN and NH₄⁺), respectively. Both COD and TN fractions for Valladolid
 436 are summarized in Table 3. This influent fractionation procedure provides a basis to synthesize and design
 437 optimal plant layout and further to robustify the solution by carrying out an uncertainty analysis, which is
 438 the last step of the developed methodology. It is essential to highlight here that the Valladolid wastewater
 439 influent is relatively diluted (i.e., low COD and TN concentration) compared to the Avedøre and Lynetten
 440 WWTPs.

441 A database consisting of capital and operating costs of each technology and their design and operational
 442 parameters is developed by referring to design handbooks, literature (Metcalf and Eddy, 2003; WEF, 2018)
 443 and a commercial database (CapdetWorks 4.0). The inventories database consisting of cost information of
 444 various technology presented in Table S2 (see SI) is reused here. The model library is customized by

³ BIOFOS 2017 annual report (https://biofos.dk/wwwroot/media/1161/2017_biofos_aarsberetning.pdf)

⁴ Personal communication

including diverse alternative technologies classified in six different treatment tasks: carbon diversion, nutrient removal, sludge thickening, supernatant or reject water treatment, and sludge dewatering. The objective of the carbon diversion task is to ensure efficient carbon removal from mainstream to the AD. This is quite crucial from an energy recovery point of view as higher carbon removal leads to higher biogas production in the AD (Behera et al., 2018; Wan et al., 2016). So for that reason, a combination of conventional technology (namely *PC* and *HRAS*) and emerging technology (such as *RBF* and *ERBF*) is considered. Likewise, for nutrient removal, both traditional activated sludge technology (i.e., *MLE*) and Anammox technology (such as *IFAS* and *ELAN*) are considered. The Anammox based technology is known for its low aeration energy requirement by following the partial nitrification mechanism (Chatterjee et al., 2016; Hoekstra et al., 2019; Malovanyy et al., 2015a; Morales et al., 2013).

Similarly for the sludge digestion, the AD is considered. A sludge thickener and a dewatering unit are also considered to handle the sludge thickening and dewatering tasks, respectively. The reject water which is generated from the dewatering unit contains 15 - 20% of the entire plant nitrogen load (Fux et al., 2002) and is often recirculated to the mainstream. However, in recent years this stream is being treated more and more frequently by using Anammox technology (Lackner et al., 2014). So for these case studies a granule based Anammox technology (*ELAN*) is considered. The mechanisms and the mathematical models for the above-mentioned technologies are explained in Table 2.

Figure 4 Superstructure representing the design space considering diverse technologies developed for the Avedøre, Lynetten and Valladolid wastewater treatment plant case studies

3.4. Dimensioning of technology alternatives

Dimensioning of primary treatment alternatives

For the given influent load and characteristics, each unit is dimensioned. For the primary treatment alternatives, such as PC, RBF, ERBF, and HRAS, the basic design dimensions mainly area and volume of the tank are calculated using the design samples generated by the Monte Carlo procedure (as explained above) and the design equations as discussed earlier. For the Avedøre influent, the volume of the PC (using Equations 1-2) can vary from 4,406 – 11,526 m³. Likewise, for Lynetten, it can vary from 9,942 – 26,002 m³ and for Valladolid in the range of 13,056 – 34,149 m³. Since the influent flow rate to the Valladolid plant is significantly higher compared to the other plants (see Table 3), this is reflected in the volume requirement. Emerging technologies like RBF and ERBF, which work based on sieving filtration techniques, are efficient to divert more carbon from the mainstream to a sidestream. In the case of ERBF, an additional tank (i.e., flocculation tank) is built before the RBF to enhance the solid separation by the filter media. So for the Avedøre influent, the volume requirement for the RBF is 147 m³ (calculated using Equations 3-4) and the ERBF is around 922 m³. Similarly, for the Lynetten and Valladolid influent, the volume requirement of the RBF is 332 m³ and 436 m³, respectively. For ERBF, the volume requirements are 2081 m³ (for Lynetten) and 2732 m³ (for Valladolid). Similarly, the HRAS works at short HRT and SRT to facilitate biosorption, and its configuration consists of an aerobic tank and a settler to separate the suspended solids. Using Equation 5, the total volume is calculated, which varies in the range of 2,413 – 4,852 m³ (for Avedøre), 5,445 – 10,959 m³ (for Lynetten) and 7,137 – 14,362 m³ (for Valladolid).

Dimensioning of secondary treatment alternatives

For the secondary treatment, technologies like MLE, IFAS, and ELAN are considered. The MLE is a conventional activated sludge process which contains an anoxic tank (for denitrification), an aerobic tank (for COD oxidation and nitrification) and a clarifier (for separating suspended biomass). Following Equations 6-8, the total volume of the MLE is estimated to be 26,961 – 103,163 m³ (for Avedøre), 60,805-232,678 m³ (for Lynetten) and 79,884 – 305,693 m³ (for Valladolid). Likewise, the IFAS and ELAN are Anammox based technologies and operates partly with a partial nitrification and partly with denitrification mechanism at low temperature. The IFAS reactor, which consists of an aerobic tank and a sedimentation tank operates in continuous mode, and K₁ type carriers are used to retain a high biomass concentration inside the aerobic tank. Using Equations 1, 2 and 10 the total volume of IFAS is determined: 36,132 – 137,568 m³ (for Avedøre), 87,005 – 346,804 m³ (for Lynetten), 91,599 – 359,864 m³ (for Valladolid). Unlike IFAS, the ELAN operates in sequential batch mode and uses granules to maintain a higher biomass

concentration inside the reactor. Since the wastewater flow rate is high in the mainline, multiple ELAN reactors can be arranged in parallel or stack manner based on the availability of civil engineering advancement (Cabrera Jr et al., 2011). Applying Equation 9, the volume of mainstream ELAN is approximated to 8,537 – 77,103 m³ (for Avedøre), 24,140 -208,187m³ (for Lynetten) and 10,178 – 159,015 m³ (for Valladolid).

Dimensioning of sludge stabilization alternatives

The sludge coming from primary and secondary treatment is further thickened and treated in AD units which operate in CSTR mode. Applying Equation 11, the volume of the AD tank is calculated to 1,216 – 17,808 m³ (for Avedøre), 3,074 – 35,534 m³ (for Lynetten) and 2,404 – 40,473 m³ (for Valladolid).

Dimensioning of sidestream treatment alternatives

The reject water which comes out after dewatering is highly concentrated in TN and the C/N ratio is low and suitable for implementing Anammox technology. In this study, ELAN technology is considered for enabling the anammox process. The major difference between mainstream and sidestream ELAN technology dimensioning is the value of NLR range (see Table S3) which reflects in the calculated volume range. Using Equation 9, the volume of sidestream ELAN is approximated to 420 – 18,058 m³ (for Avedøre), 1,049 – 42,511m³ (for Lynetten) and 1,289 – 51,701 m³ (for Valladolid).

Dimensioning of base case plant layout

As shown in Figure 3, all the three plants use a PC for the primary treatment task, the activated sludge process for the secondary treatment task, a thickener, AD and a dewatering system are used to reduce the sludge volume and produce biogas as primary energy recovery medium. The supernatant water is recycled back to the primary clarifier. The purpose of designing the base case plant layout is to compare with the potential plant layouts proposed by the integrated methodology (discussed in a later section). It is essential to mention here that the detailed design data of the real plant was not accessible, and therefore each unit of the base case plant layout is designed for each influent wastewater type (Avedøre, Lynetten, and Valladolid) using the above-explained procedure. An example of Avedøre WWTP is presented in SI.5 (see SI).

525**4. RESULTS AND DISCUSSION**

526 Applying a combinatorial approach to the customized technology library, multiple plant layouts are
527 generated (see Figure 4). So, in total, there are 320 layouts and each layout to be simulated with 100
528 different design parameters sampled using the Monte Carlo procedure. Since the primary objective is to
529 maximize energy recovery, using process knowledge, unrealistic layouts (for example layouts without AD
530 unit) are eliminated before simulation which help to reduce the number of simulations from 32,000 to
531 24,000 for each influent wastewater type. Since the methodology uses computational demanding consensus
532 models, a systematic initialization strategy (see Figure 2) is applied to initialize each unit of the plant
533 layout. Daily average influent load values (as presented in Table 3) are used to perform plant-wide
534 simulations in the MATLAB-Simulink (2017a) environment. Since many process models equations are
535 highly nonlinear and mainly based on ODEs and PDEs, a stiff solver like ODE15s is preferred. To better
536 manage the computational budget, each model equation script is written in the C language, and the parallel
537 computing features of MATLAB are exploited. The simulation results are presented in a parallel plot (see
538 Figure 5) to visualize all the layouts (both feasible and unfeasible) and their corresponding design
539 performance. In the parallel plot the feasible plant layouts (green lines in Figure 5) are filtered by applying
540 effluent constraints (i.e., COD < 100 g COD/m³, TN < 10 g N/m³ and NH₄⁺ < 1 g N/m³) as explained earlier.

541
542 *Figure 5 Displaying feasible plant layout (in green), unfeasible plant layout (in grey) and effluent constraints (in magenta) with*
543 *key performance indicators generated from Monte Carlo simulations for the Avedøre influent.*

544

4.1. Deterministic plant layouts and their design selection

Objective 1: Building an energy recovery plant

Since the primary objective is to maximize energy recovery, the optimization problem is formulated as a single objective problem, as presented in Table S13 (see SI). The NER is calculated (see Equations S1-S3) by subtracting the plant-wide energy consumption (accounting mainly for aeration, mixing and heating) from the total energy production (in the form of heat and electricity) by combustion of the methane gas from anaerobic digester in a CHP facility.

From Table 4, it is clear that the Lynetten wastewater influent has the highest theoretical energy potential (considering 1 kg COD ~ 2.73 kwh for Avedøre and Valladolid WWTP, 1 kg COD ~ 4.03 kwh for Lynetten WWTP, see SI.3 for details) to recover as the concentration of COD is relatively higher than the influent of the other plants (see Table 3). The Lynetten plant recovers energy in the form of heat only, whereas the other two plants recover energy in the form of electricity and heat. For each influent type, the top-ranked plant layout proposed by the integrated methodology recovers more energy (see Table 4) than the existing plant layout (i.e., base case). For example, in the case of Avedøre influent, the top plant layout (i.e., *HRAS-IFAS-TH-AD-DW*) recovers 16% more energy than the existing plant layout. Likewise, for Valladolid wastewater influent, the existing plant layout consumes more energy than it produces. Whereas, the top ranking plant layout (i.e., *HRAS-MLE-TH-AD-DW*) proposed by the integrated methodology recovers 24% more energy than the base case. This was possible because the PC unit (i.e., primary treatment) of the existing plant layout is retrofitted with a HRAS unit, which provides an advantage to divert more carbon to the AD compared to the base case layout. Since the Valladolid wastewater influent is diluted in terms of COD concentration and the ratio of pCOD to sCOD is also low (see Table 3), the PC which works based on gravity settling could not compete with HRAS which works based on biosorption (efficient at removing both soluble and particulate COD). Moreover, the energy consumption of the HRAS is lower compared to the PC as it operates at a very low DO set point thus avoiding excessive oxidation of COD (Jimenez et al., 2015).

For both the Avedøre and Lynetten WWTPs, a combination of HRAS as primary treatment technology and IFAS as secondary treatment technology is a top choice to maximize the NER. Interestingly, for the Valladolid wastewater influent, the methodology picks the HRAS and MLE combination. This could be because the influent wastewater for the Valladolid plant has a lower TN concentration (see Table 3) compared to the other two plants, and this does not limit the MLE performance on nitrogen removal (see Table 4) although stringent effluent concentration constraints are imposed. Moreover, external carbon is

also added to MLE for better denitrification. The net energy recovery of the Lynetten plant is highest among the three plants since the COD mass present in the Lynetten influent is relatively higher (see Table 3 and Table 4) and selecting HRAS as primary treatment alternative ensures efficient carbon diversion to the AD unit. For the primary treatment task, ERBF is ranked as the second choice after HRAS as the addition of polymer improves the suspended solids removal due to coagulation and flocculation mechanisms. It is also evident from the results summary (i.e., Table 4) that sidestream treatment by ELAN technology helps to achieve a higher energy recovery as it works based on the partial nitrification mechanism and needs comparatively less aeration energy than complete nitrification (Lackner et al., 2014). Overall, these outcomes demonstrate that the simulation-based optimization methodology can intelligently select technologies based on geographical location and priorities.

586

587 Table 4 Summary of deterministic solution for building energy recovery plants (objective 1) for Avedøre, Lynetten, and Valladolid wastewater influent. A negative value of the
 588 objective function means that the plant consumes more energy than it produces.

Plant	Process flow diagram	Energy recovery potential (MWh/d)	Estimated energy recovery (MWh/d)		Net energy recovery (%)	OBJ function (MWh/d)	Ranking
			Heat (MWh/d)	Electricity (MWh/d)			
Avedøre	<i>PC-MLE-TH-AD-DW (Base case)</i>	93.56	20.57	16.16	9%	8.29	-
	HRAS-IFAS-TH-AD-DW (L1)	93.56	23.56	18.51	25%	23.74	1
	HRAS-IFAS-TH-AD-DW-ELANS (L2)	93.56	21.86	17.18	23%	21.92	2
	ERBF-MLE-TH-AD-DW (L3)	93.56	20.33	15.97	12%	11.65	3
	ERBF-ELANM-TH-AD-DW-ELANS (L4)	93.56	16.88	13.26	11%	10.26	4
	ERBF-IFAS-TH-AD-DW-ELANS (L5)	93.56	17.42	13.69	10%	8.95	5
Lynetten	<i>PC-MLE-TH-AD-DW (Base case)</i>	430.16	180.97	0.00	24%	101.69	-
	HRAS-IFAS-TH-AD-DW (L1)	430.16	203.71	0.00	35%	152.09	1
	HRAS-IFAS-TH-AD-DW-ELANS (L2)	430.16	189.26	0.00	32%	139.23	2
	ERBF-MLE-TH-AD-DW-ELANS (L3)	430.16	176.87	0.00	27%	118.13	3
	ERBF-MLE-TH-AD-DW (L4)	430.16	171.34	0.00	25%	108.45	4
	ERBF-IFAS-TH-AD-DW (L5)	430.16	155.18	0.00	22%	93.88	5
Valladolid	<i>PC-MLE-TH-AD-DW (Base case)</i>	211.49	38.07	29.91	-9%	-19.62	-
	HRAS-MLE-TH-AD-DW (L1)	211.49	48.22	37.89	14%	28.63	1
	HRAS-IFAS-TH-AD-DW (L2)	211.49	40.26	31.64	11%	22.92	2
	HRAS-IFAS-TH-AD-DW-ELANS (L3)	211.49	34.85	27.38	7%	13.93	3
	ERBF-IFAS-TH-AD-DW (L4)	211.49	39.55	31.07	1%	2.18	4
	ERBF-MLE-TH-AD-DW-ELANS (L5)	211.49	39.48	31.02	1%	1.18	5

589

590

591 Figure 6 Comparison of key performance indicators (for objective 1) among the top five plant layouts and base case plant layout of (a) Avedøre (b) Lynetten (c) Valladolid WWTP

Objective 2: Building an economically sustainable energy recovery plant

For the second objective, there are three significant priorities, which are cost, sustainability, and energy recovery. Here the cost accounts for both capital cost (mainly equipment and construction) and operational (such as electricity, chemicals, etc.) cost. The problem is treated as multi-objective optimization (see Table S13) where the NER needs to be maximized, and the other two objectives need to be minimized. A weight-based multi-criteria strategy is applied to find optimal solutions for each influent wastewater. Before that, each objective is normalized (using a min-max approach) between 0 to 1, and equal weights are assigned ($w_1 = w_2 = w_3 = 0.33$). These weights are flexible to change based on user priorities.

$$J = w_1.NER - w_2.GHG_s - w_3.TAC$$

17

Figure S4 and Table S14 (see SI) summarise the comparison of potential plant layouts performance against the base case design of three different influents. Key findings are as follows:

- To build an economically sustainable energy recovery plant, the layout *HRAS – IFAS – TH – AD – DW* is the top choice identified by the methodology irrespective of the influent. This highlights that the combination of efficient carbon recovery with mainstream Anammox technology can be a promising one to build economical sustainable energy recovery WWTPs. Apart from that, other units such as ERBF (uses a polymer to enhance carbon diversion) and ELAN are also promising alternatives.
- Plant layout including the MLE unit is not favorable for building an economical sustainable energy recovery factory as it emits a high quantity of GHGs compared to the other secondary treatment units (see Figure S4) and the capital cost is significantly higher as well (see Table S2). Studies (Campos et al., 2016; Okabe et al., 2011) also confirm that the mainstream Anammox process emits less N₂O gas.
- For the Valladolid influent, other plant layouts (except top 1) have a negative NER value, which means the plant consumes more energy than it can produce. Moreover, the net energy recovery by the top ranking plant layout is approximately 11 %, which is low compared to the other two plants. This is because the Valladolid influent wastewater has a comparatively low COD concentration, which is a critical bottleneck for harvesting surplus energy. The current practice in the Valladolid WWTP is to import external sludge/food waste to the AD unit to enhance biogas production.

620

621 **4.2. Stochastic analysis of selected plant layouts and respective designs**

622 The plant layouts chosen in the previous step (i.e., step 5) are selected based on a yearly average influent
623 load which is subjected to change due to population growth, climate change, etc. Moreover, in practice the
624 influent load to the WWTP changes daily/weekly/monthly. Therefore it is critical to ensure that the plant
625 layout proposed by the integrated methodology should be robust to handle unforeseen events. In this
626 context, uncertainty in the influent wastewater is used as a basis to perform stochastic analysis on selected
627 plant layouts resulting from the deterministic analysis (i.e., step 5) and has also been used in other studies
628 (Al et al., 2019b; Bozkurt et al., 2016; Castillo et al., 2016a; Sin et al., 2009).

629 *Uncertainty characterization*

630 In the three WWTP influent, mainly COD and ammonium are considered to vary, and their upper and lower
631 bounds are defined in Table S15. Since the actual distribution of the considered influent fractions is not
632 known, a uniform probability distribution is assigned to each component. Furthermore, a 30% variation
633 around the deterministic value was assumed for these components. The Latin Hypercube Sampling (LHS)
634 technique with no correlation among the components is used to sample the distribution, and the sample size
635 is limited to 100. The biodegradable particulates (X_S) fraction is estimated by subtracting the sum of S_S , X_I ,
636 and S_I from the total influent COD to ensure that the COD mass balance is respected.

637 The selected top five plant layouts in the deterministic analysis (i.e., step 5) are further simulated using the
638 Monte Carlo technique to quantify the uncertainty on the objective functions under influent uncertainties.
639 The results of all the three plants are presented in terms of mean and 95% confidence interval for each
640 objective function to redefine the ranking based on the stochastic analysis.

641 *Ranking of promising plant layouts including uncertainty for objective 1*

642 The objective is to build an energy recovery plant for each influent wastewater. Therefore the performance
643 of a layout is ranked based on the mean value of the NER (generated from stochastic analysis). While
644 ranking, it is assumed that a layout having more than 20% effluent constraint violations should be given
645 less priority. Table 5 and Figure 7 summarize the stochastic analysis results, which are discussed as
646 follows:

- For Avedøre and Lynetten influent, some potential plant layouts (for example *HRAS - IFAS - TH - AD - DW*) selected in the deterministic step are not able to handle the influent uncertainty, whereas it works well for the Valladolid influent. This could be because of the relatively diluted influent wastewater for the Valladolid WWTP (see Table 3) which does not put any extra stress on the plant.
- Stochastic analyses reveal (based on Avedøre and Lynetten results) that the plant layout promising a high energy recovery may not always respect the effluent discharge regulations.
- For the Avedøre and Lynetten WWTP, stochastic analysis suggests that sidestream treatment with Anammox technology (i.e., ELAN) should be considered to handle the uncertainty in the nitrogen load better.
- The energy recovery after stochastic analyses steps is further reduced compared to the deterministic analyses, which is mainly due to the variation in influent COD load. This demonstrates the importance of evaluating influent uncertainties on the potential energy recovery.
- Stochastic ranking differs from the deterministic ranking, especially for Avedøre and Lynetten, which highlight its importance in the overall methodology and helps to contemplate the real situation.

663

664 Table 5 Comparison of the deterministic and stochastic ranking of potential plant layouts for building an energy recovery plant (objective 1). A negative value of the objective
 665 function means plant consumes more energy than it produces.

Plant	Process flow diagram	Deterministic objective function (MWh/d)	Deterministic ranking	Stochastic objective function .(MWh/d)	Effluent discharge violation	Stochastic ranking
Avedøre	<i>PC-MLE-TH-AD-DW (Base case)</i>	8.29	-	8.89	41%	-
	HRAS-IFAS-TH-AD-DW (L1)	23.74	1	21.08	61%	5
	HRAS-IFAS-TH-AD-DW-ELANS (L2)	21.92	2	19.27	0%	1
	ERBF-MLE-TH-AD-DW (L3)	11.65	3	9.52	0%	2
	ERBF-ELANM-TH-AD-DW-ELANS (L4)	10.26	4	9.48	1%	3
	ERBF-IFAS-TH-AD-DW-ELANS (L5)	8.95	5	8.18	0%	4
Lynetten	<i>PC-MLE-TH-AD-DW (Base case)</i>	101.69	-	104.16	42%	-
	HRAS-IFAS-TH-AD-DW (L1)	152.09	1	140.96	60%	5
	HRAS-IFAS-TH-AD-DW-ELANS (L2)	139.23	2	132.83	0%	1
	ERBF-MLE-TH-AD-DW-ELANS (L3)	118.13	3	111.39	46%	4
	ERBF-MLE-TH-AD-DW (L4)	108.45	4	96.25	1%	2
	ERBF-IFAS-TH-AD-DW (L5)	93.88	5	84.20	0%	3
Valladolid	<i>PC-MLE-TH-AD-DW (Base case)</i>	-19.62	-	-17.84	9%	-
	HRAS-MLE-TH-AD-DW (L1)	28.63	1	14.31	18%	2
	HRAS-IFAS-TH-AD-DW (L2)	22.92	2	17.19	6%	1
	HRAS-IFAS-TH-AD-DW-ELANS (L3)	13.93	3	4.29	0%	3
	ERBF-IFAS-TH-AD-DW (L4)	2.18	4	0.95	0%	4
	ERBF-MLE-TH-AD-DW-ELANS (L5)	1.18	5	-0.22	4%	5

666

Figure 7 Mean value of net energy recovery (NER) of the top five ranking plant layouts and their respective 95% confidence interval (thin black bars) obtained from the influent wastewater uncertainty analysis: (a) Avedøre (b) Lynetten (c) Valladolid WWTP

Ranking of promising plant layouts including uncertainty for objective 2

Objective 2 aims to build an economical sustainable energy recovery plant, which has three priorities, namely cost (TAC), GHGs emission, and NER. Similar to deterministic analysis, the mean values of TAC, NER, and GHGs for each layout are normalized, and a weighted sum is calculated (applying Equation 17). The effluent discharge violation is relaxed up to 20% while ranking the plant layout. The key findings from Figure S5 and Figure S16 are the following:

- For Avedøre and Lynetten, a common plant layout (*HRAS – IFAS – TH – AD – DW- ELANS*) is selected by the methodology which is similar to the findings for objective 1 (see Table 5). On the other hand, for the Valladolid influent, the *HRAS – IFAS – TH – AD – DW* plant layout is selected as most promising plant layout which may be due to the low influent ammonium load (see Table S15) compared to the other influents. Therefore no sidestream treatment is required for the

Valladolid influent. Moreover, this puts further emphasis on the fact that the combination of enhanced carbon recovery technology with mainstream and sidestream Anammox technology is a suitable combination to build an energy recovery WWTP.

- Furthermore, most of the potential plant layout candidates (for the Valladolid influent) have a negative NER (see Figure S5), which means that building an economically sustainable energy recovery plant may not be a smart choice, especially when the influent wastewater is diluted in terms of COD load. To achieve a surplus energy production, the plant will need to supplement the influent COD load with external carbon sources (sludge waste, food waste, etc.).

5. CONCLUSIONS

The proposed process synthesis (SPD Lab) tool has been successfully applied to study and analyze design retrofit scenarios for three full-scale WWTPs- two from Denmark and one from Spain. The steps involved in the methodology are systematically demonstrated by formulating their realistic scenarios from designing an energy recovery plant perspective. The sole objective behind the scenario formulation is to illustrate the influence of several factors such as end-user priorities, uncertainty in the influent wastewater load, government regulation, etc. on the decision-making process. A model library incorporating diverse technologies (in total 11 technologies) combining conventional as well as emerging technologies, is applied to select and design an energy recovery plant for Avedøre, Lynetten, and Valladolid wastewater influent. In total 320 alternative plant layouts representing different combinations of treatment units are generated and rigorously simulated with 100 different design parameter sets to find the optimal plant layout for each influent type.

The key advantages of the proposed integrated methodology are: it handles a wide range of computational demanding consensus models, handles a broad range of design and operating conditions, provides higher visibility on performance at each stage (such as primary, secondary treatment, etc.) of treatment technology, calculates effluent quality indicators in a more reliable way. Major conclusions from these case studies are given below:

- Higher carbon recovery favors higher energy production. HRAS and ERBF presence in top five layouts is dominating as primary treatment alternative technology.
- For all the three influent types, higher carbon recovery technology like HRAS and ERBF are more suitable for building an energy recovery plant because higher carbon diversion leads to higher biogas production from AD.

- Along with efficient carbon recovery technology, mainstream and sidestream Anammox technology (such as ELAN and IFAS) contribute to overall energy production by significantly reducing the aeration energy demand compared to a conventional activated sludge process.
- Compared to current designs, the methodology identified optimal retrofitting solutions with promising improvements in net energy recovery (NER) as much as three folds for Avedøre and 1.5 fold increase for Lynetten WWTP. While the stochastic analysis indicated that the potential improvements are decreased, given the influent load variation, there is still a strong case for considering and pilot testing emerging concepts of carbon recovery in WWTP plants for enhancing biogas production in AD.
- The COD present in influent wastewater can be a suitable indicator for deciding whether to build an energy recovery plant or not. Compared to Danish WWTPs (Avedøre and Lynetten), the Spanish WWTP (Valladolid) has low net energy recovery because influent wastewater is diluted.
- The plant layouts proposed by the SPDLab tool ensures higher energy recovery potential, lower GHGs emission, and cost than the existing real plant layouts. Simulation-based optimization is consequently useful for taking decision intelligently by recognizing the existing variability
- Uncertainty in the influent wastewater composition greatly influences the ranking of plant layouts, which emphasizes the importance to include it in the methodology. However, it is essential to note that the uncertainty bound is highly subjective and other design inputs such as safety factor, effluent requirements, etc. as suggested by Flores-Alsina et al. (2012) should be judiciously defined.

Indeed, treatment objectives, such as micro-pollutants removal (e.g. refractory toxic organics like pharmaceuticals, pesticides, personal care products, etc.), require the adaptation of tertiary treatment techniques (membrane processes, advanced oxidation techniques, etc.) which in turn, can be adapted for different treatment objectives along the process layout (e.g. membrane assisted biological process-MBR, pre-ozonation of organics, etc.). Therefore, future work can focus on expansion of the technology library. Moreover, the deterministic (step 5) and stochastic (step 6) ranking of the proposed integrated methodology can be integrated with a multi-objective optimization solver to find optimal plant layout and designs.

7376. SOFTWARE AVAILABILITY

Availability: Development version available on GitHub

(<https://github.com/cbeh447/SPDLab1.0>)

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