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Resource recovery and wastewater treatment modelling

Kimberly Solon¹, Eveline I.P. Volcke¹, Mathieu Spérandio² and Mark C.M. van Loosdrecht^{3,*}

¹ Biosystems Control Group, Department of Green Chemistry and Technology, Ghent University, Ghent, Belgium. E-mail: kimberly.solon@ugent.be, eveline.volcke@ugent.be

² LISBP, Université de Toulouse, CNRS, INRA, INSA, Toulouse, France. E-mail: sperandio@insa-toulouse.fr

³ Department of Biotechnology, Delft University of Technology, Delft, The Netherlands. E-mail: m.c.m.vanloosdrecht@tudelft.nl

*corresponding author

Abstract: Traditional wastewater treatment plants (WWTPs) are increasingly regarded as water resource recovery facilities (WRRFs), reflecting the value of water, nutrients, energy and other resources, besides ensuring the required effluent quality. Resource recovery techniques involve biochemical, physical and physico-chemical processes, and even previously unexploited biological conversions. Biopolymers and bioplastics production also reveal the remarkable potential present in our microbial cultures. Models have demonstrated their usefulness to optimize WWTP operation to achieve better effluent quality at lower costs; they also constitute a useful tool to support the transition of WWTPs into WRRFs that maximize the valorization of products recovered from the wastewater. In this paper, it is discussed to which extent the new techniques and unit processes applied for resource recovery could be modelled with conventional activated sludge models (ASMs) and which additional modelling challenges are faced while providing recommendations of potential approaches to address current modelling research gaps..

Keywords: resource recovery, wastewater treatment, modelling, activated sludge models

1. INTRODUCTION

The goals of wastewater treatment have evolved over the years. It originated from the needs of sanitation and moved towards protecting the environment. The concept of circular economy has gained traction in the last few decades as a potential key to solving the rising scarcity of resources due to urbanization and population growth. Nonetheless, the resource recovery approach is not new (Ashley *et al.*, 2011). Actually in Prague, Amsterdam and several other European countries, the wastewater was first used as a resource for phosphate and nitrogen recovery before wastewater treatment plants were built (de Bas, 1882). Wastewater treatment came after resource recovery, and now the past is being revisited.

The type of resource recovery practiced nowadays is primarily aimed at improving the general operation of the treatment plant. An example is sludge digestion to reduce the amount of sludge in the first place and having biogas production as an on-the-side benefit. A similar example is struvite recovery, which is performed primarily to reduce the maintenance cost associated with struvite precipitation in the plant, even though utilities rather specify it is for phosphate recovery.

Activated sludge models (ASMs) (Henze *et al.*, 2000) have successfully formed the industrial standard for wastewater treatment process modelling, even though they are a simplification of reality and do not encompass all scientific knowledge. Aside from teaching and research purpose, the aim of the ASMs development was to obtain a simple model with a minimum number of parameters, which operators and designers could work with and could use to analyse wastewater treatment plants (Gernaey *et al.*, 2004). Indeed, the ASMs describe oxygen dynamics (through the COD balance) and thus aeration demands, sludge production and effluent quality in terms of COD, nitrogen and phosphorus (i.e. ASM2/2d/3). The aeration requirements, sludge production and the need for recycle

53 pump capacity are actually an outcome of ASM1. Prediction of biogas production could also be
54 included. Unit processes such as crystallizer and nanofiltration units are not covered by the ASM
55 models and would need dedicated models to describe struvite and water recovery, respectively. In all
56 cases, resource recovery models need to well describe product specifications, similar to effluent
57 characteristics for wastewater treatment models.

58
59 Resource recovery units will often be operated in relatively stable conditions and not with the same
60 dynamics as in the main water line of the treatment plant. Thus, there is less need for dynamic models
61 and stoichiometric models may be adequate enough to describe most recovery processes. However,
62 dynamic modelling are still useful for optimization, and especially when taking into account the
63 interaction of the recovery process with the rest of the wastewater treatment plant unit processes.

64
65 There might be a need to make dedicated models for dedicated processes, for instance, model for
66 design of a struvite reactor for struvite recovery. It might not be useful to make one model similar to
67 ASM1 suitable for all resource recovery options. What is needed is that these resource recovery
68 models use the same state variables such that they can be integrated for a specific site. For plant-wide
69 simulation studies, these dedicated models could be coupled with other existing models by
70 constructing model interfaces as detailed by Volcke *et al.* (2006).

71
72 Wastewater treatment plants are often considered in a larger context, including sewers supplying the
73 wastewater, water bodies to which the treated effluent is discharged and maybe even water
74 reclamation facilities. When considering resource recovery, looking beyond the fence of a wastewater
75 treatment plant is even more needed because the amount of resources a single plant can deliver is too
76 small to be recognized as a real resource factory. Wastewater handling needs to be integrated into the
77 whole urban water system, considering the interactions of the individual pieces, and this holds even

78 more true when resource recovery comes into play. Integration allows for a holistic approach to
79 management and possible cost-effective solutions (Butler & Schütze, 2005). There should be more
80 focus on models which include the economy and also life cycle analysis in the context of product
81 formation and product replacement (de Faria *et al.*, 2015).

82

83 This contribution deals with modelling needs associated with the reconfiguration of wastewater
84 treatment plants (WWTPs) into water resource recovery facilities (WRRFs). The focus lies on
85 recoverable resources that are being exploited at a large scale or at least have the potential to be so,
86 tackling a number of questions. Are the activated sludge models (ASMs) still state of the art? Are
87 they still relevant? Or should a completely different set of models be used? And which modelling
88 needs does the integration of wastewater treatment in a larger context bring about?

89

90

91 **2. RECOVERABLE RESOURCES**

92

93 **2.1. Energy**

94 **Biogas – carbon redirection**

95 In the context of resource recovery, organics in the wastewater can be considered as reservoirs of
96 energy rather than pollution. Energy generation is included and implemented in the ASMs through
97 consideration of organics measured as chemical oxygen demand (COD). Techniques such as
98 enhanced primary treatment and high-rate activated sludge systems have often been used to increase
99 the amount of organics that are sent to the anaerobic digester, wherein these organics are converted
100 to biogas (Wan *et al.*, 2016). For anaerobic digestion, the important thing is to know how much
101 biodegradable particulate COD and active biomass fraction gets out of the activated sludge because
102 those are what are converted to methane. Thus, there is no need for further complexity for the

103 anaerobic digestion models (Ekama *et al.*, 2007; Ikumi *et al.*, 2014) with regards to energy recovery.
104 Anaerobic co-digestion is also being utilised to maximize biogas production (Zaher *et al.*, 2009), but
105 problems due to pH changes can be encountered when food wastes and other types of substrates are
106 added into the digester. It should be pointed out, however, that importing food waste into the
107 wastewater treatment plant does not equate to recovery because it is not actually improving the energy
108 recovery efficiency from wastewater itself but increases the energy production by introducing an
109 external energy source (i.e. food waste). This is an action that can be done by any water utility, but it
110 is not generating new energy from the wastewater.

111

112 A-stage systems, such as high-rate activated sludge, are nowadays being explored for carbon
113 redirection (Jimenez *et al.*, 2015). There is a high variability in the efficiency of the conversion and
114 solid-liquid separation processes among the different A-stage plants. ASMs can do a very good job
115 describing high-rate systems as demonstrated by Smitshuijzen *et al.* (2016). The most important
116 aspect is to recognize that a part of the biodegradable soluble COD fraction is colloidal material which
117 will not be converted by bacteria in an A-stage but would then be removed in the settler. In this case,
118 proper wastewater characterization is essential. Nogaj *et al.* (2015) developed a modified ASM1
119 considering dual soluble substrate (i.e. fast and slow) and additional processes related to these dual
120 substrate, extracellular polymeric substances (EPS), storage products and colloidal substrate. Apart
121 from proper wastewater characterization, additional parameter estimation and validation should be
122 performed due to new included model state variables, parameters and processes. A crucial part in an
123 A-stage system is not the biological part but rather the flocculation part. The formed flocs are
124 extremely weak such that the way the inlet system to the A-stage clarifier is constructed will strongly
125 influence how and how much suspended solids will end up in the A-stage clarifier effluent (de Graaff
126 & Roest, 2012). Describing the inlet mixing phenomena as done for secondary settlers (Torfs, 2015)

127 could prove useful. This aspect of floc formation should be examined first before directing all efforts
128 to make an improved ASM for modelling A-stage systems.

129

130 **Heat recovery**

131 Arising from hot water use (e.g. for bathing, cleaning), wastewater originating from households
132 retains part of its thermal energy as it flows from the domestic source to the centralized WWTP. The
133 recovery of this thermal energy recovery can be done at the source (i.e. households or buildings),
134 along the sewer line, or at the WWTP (Cipolla & Maglionico, 2014). The greater quantity of
135 recoverable thermal energy due to larger volumetric flows and the probable negative effect on
136 treatment process efficiency when considerable amount of heat is removed upstream are the main
137 reasons why heat recovery at large-scale centralized WWTPs attracts more attention (Neugebauer *et*
138 *al.*, 2015). Heat can be recovered from the effluent, digester sludge or filtrate, or if done in a controlled
139 manner, even from the influent, through heat pumps and/or heat exchangers. The most common
140 approach, however, is utilizing combined heat and power generation units for the digester biogas.
141 The thermal energy produced by such heat pumps with wastewater as heat source are on average 3.5
142 times higher than the electrical energy required to power them (Zhao *et al.*, 2010). The recovered
143 energy can then be used for cooling/heating the office buildings in the WWTP and for process heating
144 (e.g. sludge drying) and thus, can directly offset the electricity costs related to the heating demands
145 of a WWTP, and for larger-scale heat recoveries, can even be distributed through district heating
146 systems (Funamizu *et al.*, 2001; Tillman *et al.*, 1998).

147

148 Investigating the viability of heat recovery from a WWTP evidently requires setting-up a model of
149 biochemical reactions together with heat balances considering the heat that is lost/gained through
150 air/liquid interface, that is associated with the influent and effluent flows, that is transmitted from
151 mechanical actuators, and that is transferred by conduction, convection and radiation, among others.

152 This allows prediction of temperature in the context of wastewater treatment and has already been
153 presented in several studies as mentioned in Fernández-Arévalo et al. (2014). Corbala-Robles *et al.*
154 (2016) further developed a temperature prediction model in biological reactors with attention to
155 foaming, which has been neglected in previous temperature prediction models, but when present, is
156 well known to significantly affect reactor temperature. Fernández-Arévalo *et al.* (2014) presented a
157 systematic description and calculation of heat fluxes in biochemical reactors within a plant-wide
158 model, coupling the ASM reactions and multi-phase biochemical transformations with heat balances.
159 A detailed cost analysis is essential to determine the economic viability of heat recovery, which is
160 dependent on current energy costs and the balance between energy production and energy
161 requirements (Corbala-Robles et al., 2016). The climate and local conditions of an on-site thermal
162 energy generation unit should also be analysed for applicability.

163

164 **2.2. Nutrients**

165 **Phosphate**

166 One of the most common chemical compound recovered from wastewater is struvite. It should be
167 noted that for the most part, recovering struvite is not the main goal of water utilities but rather
168 reducing the operational issues due to struvite scale formation (Parsons & Doyle, 2004). Typically,
169 the recovered struvite has not yet reached more than 25% of the influent phosphate load (Egle *et al.*,
170 2016). Processes other than struvite recovery should be considered if one is really interested in
171 phosphate recovery. Consideration of phosphate in the wastewater and its recovery involves
172 chemistry and microbiology that are more complex than what are typically included in the ASMs
173 (Hauduc *et al.*, 2015; Santos *et al.*, 2018). Phosphate chemistry can be easily included by coupling
174 ASMs with geochemical modelling software such as PHREEQC (Zhang *et al.*, 2011; Parkhurst *et al.*,
175 2013; Vaneeckhaute *et al.*, 2018) or with aqueous phase chemistry modules (Flores-Alsina *et al.*,
176 2015; Kazadi Mbamba et al., 2016; Lizarralde *et al.*, 2015).

178 It is also essential to include relevant metals in the influent, especially iron (Batstone *et al.*, 2012;
179 Flores-Alsina *et al.*, 2016; Hauduc *et al.*, 2015). Iron is quite often neglected although systems which
180 have anaerobic groundwater over the sewers often experience iron intrusion, and some other sources
181 of iron in the sewer systems. In fact, quite a number of considered bio-P treatment plants in the
182 Netherlands might achieve 20-50% chemical phosphate removal, as a result of the amount of iron in
183 the influent wastewater (Wilfert *et al.*, 2016). If the iron fraction in the influent is not taken into
184 account, the bio-P model alone is not suitable. In addition to the iron that is already included in the
185 influent, some of the externally added iron will precipitate with phosphate as vivianite. Vivianite may
186 not be directly useful in agricultural applications but is nevertheless useful for other kinds of industrial
187 processes (Wilfert, 2018) and is an approach to further increase phosphate recovery.

188

189 The challenges in recovering phosphorus from the sewage sludge through the crystallization process
190 (e.g. as struvite, vivianite) is related to the economic feasibility of the process, quality of the product
191 and technical complexity of the process (Le Corre *et al.*, 2009). Complex chemical precipitation
192 models have already been developed, effect on effluent quality of P recovery units has been evaluated
193 and the impact on operational costs has been determined. However, the existing models do not take
194 product quality yet into account.

195

196 An alternative option to recover phosphorus is through sludge incineration followed by acid
197 extraction and adsorption. The phosphate is recovered from the ashes. In this case, there is no need
198 for recovery models since ASM-based models can describe P inclusion in the sludge fraction. In a
199 study by Franz (2008), two Swiss sewage sludge ash from incineration contains as much as 4-9%
200 phosphorus. There are a lot of drivers to recover P from the ashes, such as to avert high disposal costs
201 and the cost benefit of selling the recovered phosphate.

202

203 Probably because of the complex microbial ecology (Santos *et al.*, 2018), it is still unclear how we
204 can recover phosphate in a much more significant fraction of the influent load and not just as a small
205 fraction coming after the digester. An example would be being the presence of sulfide in the influent
206 which leads to the cultivation of an organism called *Thiotrix caldifontis*. It oxidizes the sulfide and
207 gets competitive advantage over the phosphorus accumulating organisms. It is also relevant because
208 *Thiotrix caldifontis* generates more biomass per unit of volatile fatty acids and has more storage
209 capacity for the phosphates (Rubio-Rincón *et al.*, 2017). This is a relevant organism to take into
210 account if there is a desire to describe it from an academic point of view, but for real applications,
211 how to efficiently deal with this microbial diversity in a model should first be determined.

212

213 **Nitrogen**

214 The Haber-Bosch process, developed in 1909, remains today as the main procedure for ammonia
215 (NH_3) synthesis from the conversion of atmospheric nitrogen (N_2) with hydrogen (H_2). The price of
216 NH_3 is highly influenced by the cost of natural gas, from which H_2 is mainly derived and represents
217 70-90% of the cost of NH_3 production (Huang, 2007; IEA, 2007). The increasing worldwide demand
218 for nitrogen fertilizer (Erisman *et al.*, 2008) for which NH_3 is mainly manufactured, and the forecasted
219 price increase of non-renewable natural gas in the future years (EIA, 2018) could result to a
220 continuous NH_3 price increase. Despite this projection, there is no extensive recovery option for
221 nitrogen yet from the perspective of municipal WWTPs with only a small fraction of the total influent
222 nitrogen recovered from the wastewater, for instance, less than 20% through phosphate-based
223 recovery processes (e.g. struvite precipitation) (Maurer *et al.*, 2002).

224

225 A viable option would be source-separated urine (Langergraber & Muellegger, 2005; Lienert &
226 Larsen, 2009) from which nitrogen can be recovered through ion-exchange, nanofiltration, ammonia

227 stripping or struvite precipitation, to mention a few (Maurer *et al.*, 2006; Pronk *et al.*, 2006; Wilsenach
228 *et al.*, 2007). However, these and other methods are still being developed particularly for full-scale
229 applications (Maurer *et al.*, 2003). One of the few large-scale approaches on nitrogen recovery is bio-
230 drying of sludge, wherein forced aeration is used to treat and further dry the dewatered sewage sludge.
231 Nitrogen, in the form of ammonium sulfate, is then recovered from the process air through an acid
232 gas scrubbing unit (Winkler *et al.*, 2013). The amount of nitrogen in the sludge can be modelled using
233 ASM while the bio-drying process requires a simple stoichiometric model describing bio-oxidation
234 coupled with energetic balances to describe the amount of water, carbon, hydrogen, oxygen and
235 nitrogen consumed. The ammonia concentration released in the gas phase is then assessed from this
236 overall consumption (Rada *et al.*, 2007) and the amount of recovered ammonium sulfate can be
237 modelled using mass balances and gas-liquid transfer to describe gaseous ammonia absorption into
238 sulfuric acid solution or by simply taking into account average ammonia removal efficiencies of acid
239 scrubbers of 91-99% (Melse & Ogink, 2005). Vaneckhaute *et al.* (2018) developed a generic nutrient
240 recovery model (NRM) focusing on nutrient recovery following anaerobic digestion, which includes
241 dynamic models for precipitation/crystallization (for struvite fertilizer products recovery) and also
242 stripping and acidic air scrubbing (for ammonium sulfate recovery).

243

244 A prospective high value nitrogenous product is microbial protein obtained from microbial growth
245 and could be used as animal feed (Becker, 2007; Hülsen *et al.*, 2018; Matassa *et al.*, 2015; Pikaar *et*
246 *al.*, 2018). Cultivated microalgae, as used in wastewater treatment for instance, contains about 50%
247 protein as dry mass (Cai *et al.*, 2013; Rasouli *et al.*, 2018). There are several existing models
248 describing microalgal growth that choose the philosophy of the ASM models as how they have been
249 setup (Decostere *et al.*, 2013; Solimeno & García, 2017; Solimeno *et al.*, 2015; Wágner *et al.*, 2016;
250 Zambrano *et al.*, 2016). Although microbial protein production through microalgal-based wastewater
251 treatment seems promising, additional studies should be first undertaken, for example, to examine the

252 cause of the large disparities in nitrogen removal efficiencies, to evaluate the effects of wastewater
253 characteristics and microbial communities on the algal composition, to economically assess the
254 recovered microbial protein and its quality as substitute for animal and human consumption.

255

256 An extensive life cycle and economic analysis are necessary to determine the practicability of
257 incorporating nitrogen recovery processes in WWTPs since there is no current compelling reason to
258 recover such a renewable resource, aside from the foreseen increasing energy cost associated with
259 the fertilizer production using the Haber-Bosch process.

260

261 **Sulfate/Sulfur**

262 Sulfate reduction, autotrophic denitrification and nitrification (SANI) process was developed in
263 Hongkong and applied in coastal areas of China to reclaim saline water without any excessive sludge
264 discharge. ASM-based models have been developed to described this process (Lu *et al.*, 2009).
265 Sulfate is also important if phosphate chemistry is to be considered. Fe-P-S interactions are significant
266 in many redox and bio-precipitation processes (Puyol *et al.*, 2017). Aerobic sulfur transformations
267 and subsequent interactions with the phosphorus and iron cycles for sewer systems has been described
268 by Gutierrez *et al.* (2010). Similar processes has been added to ASM2d in order to describe the sulfur
269 transformations in activated sludge systems and its interactions with the phosphorus and iron cycles
270 (Solon *et al.*, 2017). Fuel gases, such as biogas obtained through anaerobic digestion, may contain
271 significant amounts of sulfur depending on the type of influent wastewater. Biogas desulfurization is
272 often performed and elemental sulfur, S⁰, can be recovered through crystallization and centrifugation
273 of the flue-gas wastewater. For this, dedicated models may be developed to describe the recovery
274 process.

275

276 **2.3. Cellulose fibres**

277 A rather often overlooked resource is fibres. In the wastewater treatment plant influent, 25-30% of
278 the COD and about 40% of suspended solids is attributed to cellulose fibres (i.e. toilet papers) (Ruiken
279 *et al.*, 2013). There are more than 300 references in wastewater characterization, however, there is
280 almost no literature on cellulose fibres and a good measurement for cellulose in wastewater or
281 activated sludge is still missing (Ruiken *et al.*, 2013), this is peculiar for such a considerable fraction
282 of the influent COD. Cellulose fibres are easy to remove and recover using only mechanical treatment
283 such as sieves. Initially used as biomass fuel for power plants, cellulose fibres are also being
284 investigated as raw material for paper products, bioplastics (van der Hoek *et al.*, 2016) and road and
285 building material. It was mentioned in a paper by Nowak *et al.* (1999) that there is a very slowly
286 degradable COD fraction in the wastewater. It is probable that this observation was due to cellulose.
287 In line with this and from the point of view of the ASMs, cellulose could simply be modelled by
288 adding a very slowly biodegradable fraction in the ASM (Reijken *et al.*, 2018). Recent modelling
289 studies pointed out the specificities of the slow hydrolysis kinetics of cellulosic solids (Beneouala *et*
290 *al.*, 2017; Lebaz *et al.*, 2015). Contrary to conventional hydrolysis in ASM, considering the specific
291 hydrolytical active biomass for such material is crucial. Another possibility is to model it as non-
292 biodegradable in high-loaded systems and biodegradable in low-loaded systems (van Loosdrecht *et*
293 *al.*, 2015). Economic assessment, energy evaluation and the effect on the overall plant efficiency of
294 integrating cellulose fibre recovery within a WWTP should be studied, taking into account whether
295 it is recovered for energy production or into another product form.

296

297 **2.4. Bioplastics**

298 Bioplastics, such as polyhydroxyalkanoates (PHAs), are produced from renewable biomass resource,
299 making it a better alternative for current petroleum-based plastics commonly in use (Możejko-
300 Ciesielska & Kiewisz, 2016; Snell & Peoples, 2009). There are microorganisms found in soil, sewage
301 and marine environments that can synthesize and accumulate PHAs. The main limitation for large

scale PHA production is the high cost which is brought about when using pure cultures (Chen, 2009; Kleerebezem & van Loosdrecht, 2007; Salehizadeh & Van Loosdrecht, 2004). A promising option, therefore, is the use of mixed cultures. However, there are still investigations on how to improve the yields from such mixed cultures (Puyol *et al.*, 2017) as it has been investigated that activated sludge can accumulate PHA up to 20-60% of the sludge dry weight (Salehizadeh & Van Loosdrecht, 2004), compared to pure cultures in which almost 90% can be achieved (Bengtsson *et al.*, 2008). PHA from mixed cultures of biomass found abundantly in full-scale municipal wastewater treatment plants is being studied in the PHARIO project in the Netherlands (Bengtsson *et al.*, 2017). However, no direct correlation between PHA accumulation potential and storage rate has yet been found in their tests. In principle, PHA accumulation can be modelled by ASM3 as demonstrated by Hanada *et al.* (2002) and Guisasola *et al.* (2005), with minor modifications to the kinetic parameters. Even more important to consider than the biokinetic modelling is the assessment of the technological, economic and environmental aspects for bioplastic production technologies, as done by Fernández-Dacosta *et al.* (2015). This multi-aspect evaluation can aid in establishing value chains for PHA production for the scale up of existing technologies.

317

318 **2.5. Extracellular polymers**

A mere 10-50% of the total organic carbon in a biofilm are cell biomass, whereas the rest can be found in the biofilm matrix (Donlan, 2002; Nielsen *et al.*, 1997). This matrix, called extracellular polymeric substances (EPS), is an aggregation of different types of biopolymers produced by microorganisms which are responsible for the structural and functional integrity of biofilms (Flemming & Wingender, 2010). Although there have been many studies of EPS characterization (Laspidou & Rittmann, 2002), detailed composition is difficult due to the complexity of the mixture (Jiao *et al.*, 2010). Moreover, their compositions vary and is determined by the origin of the biofilm and extraction mechanism (Wingender *et al.*, 1999). EPS are a potential resource of polyelectrolytes,

they can be applied for soil remediation (Jia *et al.*, 2011) as an alternative to surfactants in order to improve the water-holding capacity of soil, they can be utilized as a material to make nanocomposite materials (Tuo *et al.*, 2015) and they can also be used for metal recovery from wastewater through biosorption (Mikutta *et al.*, 2012; More *et al.*, 2014). Aerobic granular sludge has shown to contain a high amount (20-30%) of alginate-like polymers (Lin *et al.*, 2010), which could replace alginate applications. A first extraction facility is currently constructed in the Netherlands (“Neo-alginaat”, 2018). Existing ASM extensions incorporating EPS concepts have been presented by Fenu *et al.* (2010) and Xavier *et al.* (2005). Nevertheless, it remains a challenge to accurately predict the actual EPS production. To take this into account in the ASM models, one would only have to include the fraction of EPS in the total sludge, however, a standard method for extraction and measuring EPS should first be established (de Kreuk *et al.*, 2007; Felz *et al.*, 2016). Moreover, the regulation and kinetics of EPS formation by activated and granular sludge microorganisms are also still unknown.

3. THE NEED FOR INTEGRATION

The perspective on products and energy recovery at WWTPs imposes multi-objective performance assessment of process configurations and operational strategies. Methods combining dynamic modelling and life cycle assessment (DM-LCA) were recently developed (Foley *et al.*, 2010; Bisinella *et al.*, 2015; Arnell *et al.*, 2017). Such simulations include not only effluent quality but also resource efficiency and recovery, global environmental impact and operational cost, considering both direct on-site and background off-site effects. The overall benefits and limitations of energy and nutrient recovery strategies can be revealed. For instance, based on plant-wide modelling methods, changing the operational strategy to recover more bio-methane by carbon capture through chemically enhanced primary treatment has been evaluated (Arnell *et al.*, 2016; Bisinella *et al.*, 2015). Results showed that

352 increase of methane production and decrease of global warming potential can be severely
353 compensated by increased consumption of chemicals, leading to high operational cost and LCA
354 impacts like abiotic depletion of elements and fossil fuel resources.

355

356 Steady state simulations are somewhat sufficient for systematic evaluation of the life cycle inventories
357 and costs for different recovery scenarios and design of plant configurations (Foley *et al.*, 2010;
358 Khiewwijit *et al.*, 2015). However, optimization studies and gaining detailed information on
359 processes' behaviour would require dynamic simulations (Langergraber *et al.*, 2004). Also, dynamics
360 should be considered for accurate evaluation of discharge limits and greenhouse gas (GHG) emission
361 (N_2O) which are both highly influenced by daily or weekly peak load (Bisinella *et al.*, 2015; Flores-
362 Alsina *et al.*, 2014). Considering both water and sludge lines when analysing GHG emissions were
363 also shown to be important and the considerable potent environmental impact of N_2O or CH_4 emission
364 were pointed out.

365

366 The importance of plant-wide modelling and simulation for evaluating the integration of recovery
367 techniques within WWTPs should be highlighted. Plant-wide models allow analysis of the effects of
368 the recovery process on the overall plant performance, understand the interdependencies of the
369 different unit processes and provide a foundation for new plant layouts for WRRF design (Fernández-
370 Arévalo *et al.*, 2017; Khiewwijit *et al.*, 2015). Integrated modelling will certainly become even more
371 necessary if extraction facilities for the resource recovery will be added on-site of the WWTP.

372

373 Extending the boundaries of modelling tools to the overall urban wastewater management system is
374 of growing interest. Modelling alternative scenarios based on source separation (urine, black water)
375 (Wilsenach & van Loosdrecht, 2006) or decentralised systems are under development to tackle the
376 issues of end-of-pipe wastewater management in which recovery is always relatively limited (20% of

377 N and P mass flows). Using adapted framework, including influent generator, alternative scenarios
378 can be assessed, showing that more benefit would be reached by recovering fertilizer and energy from
379 undiluted streams (Ishii & Boyer, 2015; Bisinella *et al.*, 2015; Igos *et al.*, 2017).

380

381 Cost analysis models also deserve more and more attention. Whereas energy cost is generally well
382 known, the market for new valuable products like struvite or polymer can be highly dependent of
383 local situation and regulation, making the approach more speculative and uncertain for such products
384 (Gurieff & Lant, 2007). The cost saving is generally considered whereas the benefit of product sale
385 can be considered as an option. A local use or dedicated market is generally encouraged. Actually,
386 water reclamation remains the main driver in cost analysis (Igos *et al.*, 2017).

387

388 Finally, recent papers describe the feasibility of coupling DM-LCA with multi-objective optimization
389 (MOO) (Bisinella *et al.*, 2016, Arnell *et al.*, 2017). The combined frameworks (DM-LCA-MOO) can
390 be applied with three objectives: Effluent Quality Index (EQI), Operational Cost Index (OCI) and
391 environmental impacts quantified through Life Cycle Impact Assessment (LCIA). Given the
392 contradictory nature of objectives, Pareto fronts are generated through simulation, which can help
393 decision making for selecting some recovery scenarios and operational conditions. The main
394 challenges and research points of those approaches are related to uncertainties evaluation, sizing
395 choice, dynamic aspects to be considered and systems boundaries definition.

396

397

398 **4. CONCLUSIONS**

399

- Despite being a simplification of reality, the ASMs remain state-of-the-art for modelling conventional WWTP processes and can even be used to describe significant part of the resource (energy, nutrients, and other products) recovery options.
- Extensions to the ASMs (e.g. to describe cellulose and sulfur recovery) or entirely dedicated new types of models (e.g. to describe heat and struvite recovery) may be needed for dedicated processes. There is certainly a need to better understand how and what we recover at the treatment plant of a local city or a local region, and for that, different types of models could be needed for the unit processes.
- Steady state models or even just stoichiometric models can be adequate to describe most recovery processes and cost analysis. Dynamic models are useful for optimizing individual processes and gaining more insight in process behaviours.
- A good resource recovery model should be able to predict product specifications, similar as how the effluent quality is assessed for wastewater treatment models.
- As we progress towards operating resource recovery facilities, integrated models are essential to make overall balanced evaluations. These integrated models should not only describe the treatment and recovery processes, but also assess life cycle, product quality and techno-economical aspects as additional important criteria associated with product formation.

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