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Resource recovery and wastewater treatment modelling

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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. Biopolymer and bioplastic 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 wastewater. In this paper, the extent to which the new techniques and unit processes applied for resource recovery could be modelled with conventional activated sludge models (ASMs) and additional modelling challenges being faced are discussed while providing recommendations of potential approaches to address current modelling research gaps.

Water impact

Models have been successfully used in operation, design and control of wastewater treatment processes. With the increasing attention given to resource recovery from wastewater, this perspective paper discusses the extent to which the new unit processes applied for resource recovery can be modelled with conventional activated sludge models and additional modelling challenges being faced are discussed.

1 Introduction

The goals of wastewater treatment have evolved over the years. It originated from the need for 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.[1] Actually in Prague, Amsterdam and several other European countries, wastewater was first used as a resource for phosphate and nitrogen recovery before wastewater treatment plants were built.[2] 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 with 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 often specify that it is for phosphate recovery.

Activated sludge models (ASMs)[3] have successfully constituted 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 purposes, the aim of ASM 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.[4] Indeed, 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 need for recycle pump capacity are actually an outcome of ASM1. Prediction of biogas production could also be included. Unit processes such as crystallizers and nanofiltration units are not covered by ASMs and would need

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dedicated models to describe struvite and water recovery, respectively. In all cases, resource recovery models need to well describe product specifications, similar to effluent characteristics for wastewater treatment models.

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

There may be a need to make dedicated models for dedicated processes, for instance, a model for design of a struvite reactor for struvite recovery. It may not be useful to make one model similar to ASM1 suitable for all resource recovery options. What is needed is that these resource recovery models use the same state variables such that they can be integrated for a specific site. For plant-wide simulation studies, these dedicated models could be coupled with other existing models by constructing model interfaces as detailed by Volcke *et al.*[5]

Wastewater treatment plants are often considered in a larger context, including sewers supplying the wastewater, water bodies to which the treated effluent is discharged and maybe even water reclamation facilities. When considering resource recovery, looking beyond the fence of a wastewater treatment plant is even more needed because the amount of resources a single plant can deliver may be too small to be recognized as a real resource factory, for instance, in the case of bioplastics.[6] Wastewater handling needs to be integrated into the whole urban water system, considering the interactions of the individual pieces, and this holds even more true when resource recovery comes into play. Integration allows for a holistic approach to management and possible cost-effective solutions.[7] There should be more focus on models which include the economy and also life cycle analysis in the context of product formation and product replacement.[8]

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

2 Recoverable resources

2.1 Energy

Biogas – carbon redirection. In the context of resource recovery, organics in wastewater can be considered as reservoirs of energy rather than pollution. Energy generation is included and implemented in ASMs through consideration of organics measured as chemical oxygen demand (COD). Techniques such as enhanced primary treatment and high-rate activated sludge systems have often been used to increase the amount of organics that are sent to the anaerobic digester, wherein these organics are converted to biogas.[9] For anaerobic digestion, the important thing is to know how much biodegradable particulate COD and active biomass fraction gets out of the activated sludge because those are the fractions which are converted to methane. Thus, there is no need for further complexity for anaerobic digestion models[10,11] with regard to energy recovery. Anaerobic co-digestion is also being utilised to maximize biogas production (as modelled by Zaher *et al.*[12]), even though problems due to pH changes can be encountered when food wastes and other types of substrates are added into the digester. It should be pointed out, however, that importing food waste into the wastewater treatment plant does not equate to recovery because it does not actually improve the energy recovery efficiency from wastewater itself but increases the energy production by introducing an external energy source (*i.e.* food waste). This is an action that can be done by any water utility, but it does not generate additional energy from wastewater as such.

A-stage systems, such as high-rate activated sludge, are nowadays being explored for carbon redirection.[13] There is a high variability in the efficiency of the conversion and solid–liquid separation processes among the different A-stage plants. ASMs can do a very good job describing high-rate systems as demonstrated by Smitshuijzen *et al.*[14] The most important aspect is to recognize that a part of the biodegradable soluble COD fraction is a colloidal material which will not be converted by bacteria in an A-stage but would then be removed in the settler. In this case, dedicated wastewater characterization is essential. Nogaj *et al.*[15] developed a modified ASM1 considering a dual soluble substrate (*i.e.* fast and slow) and additional processes related to the dual substrate, extracellular polymeric substances (EPS), storage products and colloidal substrate. Apart from proper wastewater characterization, additional parameter estimation and validation should be performed due to new included model state variables, parameters and processes. A crucial part in an A-stage system is not the biological part but rather the flocculation part. The formed flocs are extremely weak such that the way the inlet system to the A-stage clarifier is constructed will strongly influence how and how much suspended solids will end up in the A-stage clarifier effluent.[16] Describing the inlet mixing phenomena as done for secondary settlers[17] could prove useful. This aspect of floc formation should be examined first before directing all efforts to make an improved ASM for modelling A-stage systems.

Heat recovery. Arising from hot water use (*e.g.* for bathing and cleaning), wastewater originating from households retains part of its thermal energy as it flows from the domestic source to the centralized WWTP. The recovery of this thermal energy can be done at the source (*i.e.* households or buildings), along the sewer line, or at the WWTP.[18] The larger quantity of recoverable thermal energy due to larger volumetric flows is the main reason why heat recovery at large-scale centralized WWTPs attracts more attention. Heat can be recovered from the effluent, digester sludge or filtrate through heat pumps and/or heat exchangers. Heat recovery from the influent (or in the sewer) is also possible, when done in a controlled way, to avoid negative effects on the treatment process efficiency.[19] The thermal energy produced by such heat pumps with wastewater as the heat source is on average 3.5 times higher than the electrical energy required to power them.[20] The recovered energy can then be used for cooling/heating the office buildings in the WWTP and for process heating (*e.g.* sludge drying), and thus can directly offset the electricity costs related to the heating demands of a WWTP, and can even be distributed through district heating systems for larger-scale heat recoveries.[21,22] Still, the most commonly applied approach for heat recovery at a WWTP is utilizing the calorific value of digester biogas by burning it in a boiler (only heat production) or in a combined heat and power generation unit. The recovered heat is then typically used to heat the digester.

Investigating the viability of heat recovery from a WWTP evidently requires setting-up heat balances considering the heat that is produced during biochemical reactions, that is lost/gained through the air/liquid interface, that is associated with the influent and effluent flows, and that is transmitted from mechanical actuators, among others. This allows prediction of temperature in the context of wastewater treatment which has already been sufficiently demonstrated in several studies.[23,24] Corbala-Robles *et al.*[25] extended previous temperature prediction models in biological reactors, in particular considering the effect of a foam layer, which significantly affects heat loss through the surface as a major factor influencing reactor temperature. A systematic description and calculation of heat fluxes in biochemical reactors within a plant-wide model, coupling the ASM reactions and multiphase biochemical transformations with heat balances, has also already been illustrated, *e.g.* by Fernández-Arévalo *et al.*[26] The focus should now turn to detailed cost analysis for specific case studies to determine the economic viability of heat recovery, which is dependent on current energy costs and the balance between heat production and heat requirements.[27] Not only should it be possible to use the amount of heat recovered on-site, it should also be available at the time there is a demand, since heat transport and/or storage would pose additional challenges. Aquifer thermal energy storage systems, for example, can be used to achieve on-site heat storage and recovery.[28] The heat supply and demand, influenced by climate and local conditions, should thus be analysed to determine the technical and economic feasibility of a thermal energy generation unit.

2.2 Nutrients

Phosphate. One of the most common chemical compounds recovered from wastewater is struvite. It should be noted that for the most part, recovering struvite is not the main goal of water utilities but rather reducing the operational issues due to struvite scale formation.[29] Typically, the recovered struvite has not yet reached more than 25% of the influent phosphate load.[30] Processes other than struvite recovery should be considered if one is really interested in phosphate recovery. Consideration of phosphate in wastewater and its recovery involves chemistry and microbiology that are more complex than what is typically included in ASMs.[31,32] Phosphate chemistry can be easily included by coupling ASMs with geochemical modelling software such as PHREEQC[33–35] or with aqueous phase chemistry modules.[36–38]

In view of phosphate recovery, it is essential to include relevant metals in the influent, especially iron,[31,39,40] through the use of aqueous phase chemistry and precipitation models as already demonstrated by Hauduc *et al.*,[31] Solon *et al.*[41] and Vaneeckhaute *et al.*[35] It is crucial to remark that, independent from whether this is done by coupling biochemical models with an external geochemical modelling software program or with self-coded aqueous phase chemistry and precipitation models, expert knowledge is of paramount importance to ensure that all relevant chemical components and species are accounted for. In addition, regarding the interest in vivianite (Fe(II) crystals), models for iron oxidation and reduction still need to be validated. These phenomena are kinetically limited and depend on the presence of other electron acceptors and donors. Iron is quite often neglected although sewer systems which have anaerobic groundwater intrusion result in significant iron in the influent of the WWTP. There could also be other sources of iron in sewer systems. In fact, quite a number of bio-P treatment plants in the Netherlands may achieve 20–50% chemical phosphate removal, as a result of the amount of iron in the influent wastewater.[42] If the iron fraction in the influent is not taken into account, the bio-P model alone is not suitable. In addition to the iron that is already included in the influent, some of the externally added iron will precipitate with phosphate as vivianite. Vivianite may not be directly useful in agricultural applications but is nevertheless useful for other kinds of industrial processes[43] and is an approach to further increase phosphate recovery.

The calibration of hydrolysis parameters for different organic phosphorus fractions during anaerobic digestion also needs more attention. This will lead to better prediction of the quantity of recoverable phosphorus in the digestate. However, the main challenges in recovering phosphorus from the sewage sludge through the crystallization process (*e.g.* as struvite or vivianite) are related to the economic feasibility of the process, quality of the product and technical complexity of the process.[44] Complex chemical precipitation models have already been developed, their effect on the effluent quality of P recovery units has been evaluated and their impact on operational costs has been determined. However, the existing models do not yet take product quality into account. The presence of other ions and the process parameters (*e.g.* pH, temperature, and mixing conditions) affect crystallization growth rates and therefore crystal size distributions.[44] These relations should be included in the existing models if product quality is to be predicted.

An alternative option to recover phosphorus is through sludge incineration followed by acid extraction and adsorption. The phosphate is recovered from the ashes. In this case, there is no need for recovery models since ASM-based models can describe P inclusion in the sludge fraction. In a study by Franz,[45] ash from incinerated sewage sludge was found to contain as much as 4–9% phosphorus. There are a lot of drivers to recover P from the ashes, such as to avert high disposal costs and the cost benefit of selling the recovered phosphate.[30]

Probably because of the complex microbial ecology,[32] good models that incorporate the microbial diversity are still lacking. Fermentative putative polyphosphate-accumulating organisms (PAOs) such as *Tetrasphaera* sp. and other recently described PAOs could give a better prediction of the polyphosphate accumulation capacity in sludge. Another example would be the presence of sulfide in the influent which leads to the cultivation of an organism called *Thiothrix caldifontis*. It oxidizes the sulfide and gets a competitive advantage over PAOs. This is relevant because *Thiothrix caldifontis* generates more biomass per unit of volatile fatty acids and has more storage capacity for phosphates.[46] A good balance between practical relevance and academic rigorousness needs to be established for these complex microbial ecosystem models.

Finally, the combination of physical–chemical and biological P removal is frequently used in WWTPs. As a consequence, models combining biological reactions and metal behaviour would need more attention in the future. Such models are needed to be able to predict the appropriate phosphorus recovery route (struvite or vivianite).

Nitrogen. The Haber–Bosch process, developed in 1909, remains today as the main procedure for ammonia (NH_3) synthesis from the conversion of atmospheric nitrogen (N_2) with hydrogen (H_2). The price of NH_3 is highly influenced by the cost of natural gas, from which H_2 is mainly derived and represents 70–90% of the cost of NH_3 production.[47,48] The increasing worldwide demand for nitrogen fertilizers[49] for which NH_3 is mainly manufactured, and the forecasted price increase of non-renewable natural gas in the future years[50] could result in a continuous NH_3 price increase. Despite this projection, there is no extensive recovery option for nitrogen yet from the perspective of municipal WWTPs with only a small fraction of the total influent nitrogen recovered from wastewater, for instance, less than 20% through phosphate-based recovery processes (*e.g.* struvite precipitation).[51]

A viable option would be source-separated urine[52,53] from which nitrogen can be recovered through ion-exchange, nanofiltration, ammonia stripping or struvite precipitation, to mention a few.[54–56] However, these and other methods are still being developed particularly for full-scale applications.[57] One of the few large-scale approaches for nitrogen recovery is bio-drying of sludge, wherein forced aeration is used to treat and further dry the dewatered sewage sludge. Nitrogen, in the form of ammonium sulfate, is then recovered from the process air through an acid gas scrubbing unit.[58] ASMs can be used to monitor the transformations of nitrogen compounds in water and their fate in the sludge line, while dedicated models can be developed and used to describe the recovery process. Indeed, the amount of nitrogen that ends up in the sludge can be modelled using an ASM while the bio-drying process requires a simple stoichiometric model describing bio-oxidation coupled with heat balances to describe the amount of water, carbon, hydrogen, oxygen and nitrogen consumed.[59] The ammonia concentration released in the gas phase can be determined from this stoichiometric model and the amount of recovered ammonium sulfate can be modelled using mass balances and gas–liquid transfer to describe gaseous ammonia absorption into sulfuric acid solution or by simply taking into account average ammonia removal efficiencies of acid scrubbers of 91–99%.[60] Vaneeckhaute *et al.*[35] developed a generic nutrient recovery model (NRM) focusing on nutrient recovery following anaerobic digestion, which includes dynamic models for precipitation/crystallization (for struvite fertilizer product recovery) and also stripping and acidic air scrubbing (for ammonium sulfate recovery). Prior to recovery, investigation is also needed to determine the factors influencing organic nitrogen mineralization into ammonium, particularly if codigestion is employed.

A prospective high value nitrogenous product is microbial protein obtained from microbial growth and could be used as animal feed.[61–64] Cultivated microalgae, as used in wastewater treatment for instance, contains about 50% protein as dry mass.[65,66] There are several existing models describing microalgal growth that choose the philosophy of ASMs on how they have been setup.[67–71] Although microbial protein production through microalgal-based wastewater treatment seems promising, additional studies should be first undertaken, for example, to examine the cause of the large disparities in nitrogen removal efficiencies, to evaluate the effects of wastewater characteristics and microbial communities on the algal composition, and to economically assess the recovered microbial protein and its quality as a substitute for animal and human consumption.

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

Sulfate/sulfur. The sulfate reduction, autotrophic denitrification and nitrification (SANI) process was developed in Hong Kong and applied in coastal areas of China to reclaim saline water without any excessive sludge discharge. ASM-based models have been developed to describe this process.[72] Sulfate is also important if phosphate chemistry is to be considered. Fe–P–S interactions are significant in many redox and bio-precipitation processes.[73] Aerobic sulfur transformations and subsequent interactions with the phosphorus and iron cycles for sewer systems have been described by Gutierrez *et al.*[74] Similar processes have been added to ASMs (and ASM-type models) in order to describe the sulfur transformations in activated sludge systems and its interactions with the phosphorus and iron cycles.[41,75] Fuel gases, such as biogas obtained through anaerobic digestion, may contain significant amounts of sulfur depending on the type of influent wastewater. Biogas desulfurization is often performed and elemental sulfur, S°, can be recovered through crystallization and centrifugation of flue-gas wastewater. For this, dedicated models may be developed to describe the recovery process.

2.3 Cellulose fibres

A rather often overlooked resource is fibres. In the wastewater treatment plant influent, 25–30% of the COD and about 40% of suspended solids are attributed to cellulose fibres (*i.e.* toilet papers).[76] There are more than 300 references in wastewater characterization, however, there is almost no literature on cellulose fibres and a good measurement for cellulose in wastewater or activated sludge is still missing,[76] which is peculiar for such a considerable fraction of the influent COD. Cellulose fibres are easy to remove and recover using only mechanical treatment such as sieves. Initially used as biomass fuel for power plants, recovered cellulose fibres are also being investigated as raw materials for paper products, bioplastics[77] and road and building materials. It was mentioned in a paper by Nowak *et al.*[78] that there is a very slowly degradable COD fraction in wastewater. It is probable that this observation was due to cellulose. In line with this and from the point of view of ASMs, cellulose could simply be modelled by adding a very slowly biodegradable fraction in the ASM.[79] Recent modelling studies pointed out the specificities of the slow hydrolysis kinetics of cellulosic solids.[80,81] In contrast to conventional hydrolysis in ASMs, considering the specific hydrolytic active biomass for such a material is crucial. Another possibility is to model it as non-biodegradable in high-loaded systems and biodegradable in low-loaded systems.[82] Economic assessment, energy evaluation and the effect on the overall plant efficiency of integrating cellulose fibre recovery within a WWTP should be studied, taking into account whether it is recovered for energy production or into another product form.

2.4 Bioplastics

Bioplastics, such as polyhydroxyalkanoates (PHAs), are produced from renewable biomass resources, making them a better alternative to current petroleum-based plastics commonly in use.[83,84] There are microorganisms found in soil, sewage 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 by using pure cultures.[85–87] 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[73] as it has been reported that activated sludge can accumulate PHA up to 20–60% of the sludge dry weight,[87] compared to pure cultures in which almost 90% can be achieved.[88] 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.[89] However, no direct correlation between the 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.*[90] and Guisasola *et al.*,[91] 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.*[92] This multi-aspect evaluation can aid in establishing value chains for PHA production for the scale-up of existing technologies.

2.5 Extracellular polymers

A mere 10–50% of the total organic carbon in a biofilm is cell biomass, whereas the rest can be found in the biofilm matrix.[93,94] 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.[95] Although there have been many studies of EPS characterization,[96] identifying their detailed composition is difficult due to the complexity of the mixture.[97,98] Moreover, their compositions vary and are determined by the origin of the biofilm and by the extraction method used preceding their identification.[99] EPS are a potential resource of polyelectrolytes. They can be applied for soil remediation[100] 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[101] and they can also be used for metal recovery from wastewater through biosorption.[102,103] Aerobic granular sludge contains a high amount (20–30%) of EPS that have alginate-like properties,[104] which could replace alginate applications. A first extraction facility is currently constructed in the Netherlands.[105] Existing ASM extensions incorporating EPS concepts have been presented by Fenu *et al.*[106] and Xavier *et al.*[107] Nevertheless, it remains a challenge to accurately predict the actual EPS production. To take this into account in ASMs, 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.[98,108,109] Moreover, the regulation and kinetics of EPS formation by activated and granular sludge microorganisms are also still unknown.

2.6 Summary

Listed in Table 1 is the summary of fundamental modelling concepts for each resource discussed in this paper and recommendations on how to address the associated needs. These are not solely recommendations directly related to modelling but also include recommendations on focus of

Table 1 Key concepts for resource recovery modelling and recommendations on associated future research and modelling efforts

Recoverable resource	Key concepts to be modelled	Recommendations – priority research topics
Energy		
Biogas	Energy content of wastewater (organics) measured as COD, more specifically biodegradable particulate COD and active biomass fractions, which are converted to methane during anaerobic digestion	Dedicated influent characterization
	The capture of COD in the produced sludge and effluent of the A-stage	Colloidal fraction consideration
		Flocculation and floc settling, affected by *e.g.* inlet mixing phenomena for A-stage clarifiers
		Parameter estimation and validation for A-stage models (bioreactor + settler)
Heat	Heat balances for temperature prediction	Cost analysis
	Economic viability of heat recovery	Balancing between heat recovery and on-site or off-site heat demand
Nutrients		
Phosphate	Phosphorus-related microbial ecology and chemistry	Include the appropriate level of microbial diversity in models
	Interaction of phosphorus with sulfur and iron	Coupling P-models with aqueous phase chemistry and precipitation models including S and Fe (model validation)
		Consider oxidation and reduction of metals involved in P recovery
		Better assessment of organic P mineralization in digesters
		Include product quality in existing phosphorus recovery models
		Life cycle analysis and cost analysis
Nitrogen	Amount of recoverable nitrogen in the sludge	ASMs
		Factors affecting organic N mineralization during anaerobic (co-)digestion
	Unit processes for nitrogen recovery (*e.g.* ammonia stripping, struvite precipitation, ion exchange, and nanofiltration)	Develop dedicated models for N recovery
	Nitrogen recovery as microbial protein	Factors influencing N removal efficiencies of microalgal-based wastewater treatment
		Life cycle analysis and cost analysis of N recovery in different product forms
Sulfate/sulfur	Sulfur biological and/or chemical transformations (oxidation and reduction) during wastewater treatment	Coupling S-models with aqueous phase chemistry and precipitation models including P and Fe (model validation)
	When applicable, consider interactions with phosphorus and iron	
	Unit processes for sulfur recovery	Develop dedicated models for S recovery, considering which form of sulfur to be recovered

Table 1 *(continued)*

Recoverable resource	Key concepts to be modelled	Recommendations – priority research topics
Cellulose fibres	Biodegradation kinetics of cellulose	Characterize cellulose fibres in wastewater
		Consider specific hydrolytic biomass for cellulosic solids in ASMs
	Economic viability of cellulose recovery	Assess the costs, energy and effect on plant efficiency when integrating cellulose recovery either for energy production or as a raw material for other products
Bioplastics	PHA yield in mixed cultures	Modelled with ASM3
		Experimental work for optimizing the PHA yield
		Life cycle analysis and cost analysis to assist in creating value chain and scale up of PHA production technologies
Extracellular polymers	EPS formation during wastewater treatment	Establish a standard method for extraction and measurement of EPS
		Investigate kinetics of EPS formation in activated and granular sludge

future research on resource recovery, which will impact and/or require modelling efforts.

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.[110–112] 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.[111,113] Results showed that positive effects such as increased production of methane as a renewable energy source, saving on CO_2 emissions and thus decreasing the carbon footprint of the plant, can be severely offset by increased consumption of chemicals, leading to high operational costs and LCA impacts like abiotic depletion of elements and fossil fuel resources.

Steady state simulations are typically sufficient for systematic evaluation of the life cycle inventories and costs for different recovery scenarios and design of plant configurations.[110,114] However, optimization studies and gaining detailed information on processes' behaviour would require dynamic simulations.[115] Also, dynamics should be considered for accurate evaluation of discharge limits and greenhouse gas (GHG) emissions (N_2O) which are both highly influenced by daily or weekly peak loads.[111,116] Considering both water and sludge lines when analysing GHG emissions was also shown to be important and the considerable potent environmental impact of N_2O or CH_4 emission was pointed out.

The importance of plant-wide modelling and simulation for evaluating the integration of recovery techniques within WWTPs should be highlighted. Plant-wide models allow analysis of the effects of the recovery process on the overall plant performance, help understand the interdependencies of the different unit processes and provide a foundation for new plant layouts for WRRF design.[114,117] Integrated modelling will certainly become even more necessary if extraction facilities for resource recovery will be added on-site of the WWTP.

Extending the boundaries of modelling tools to the overall urban wastewater management system is of growing interest. Modelling alternative scenarios based on source separation (urine or black water)[118] or decentralised systems are under development to tackle the issues of end-of-pipe wastewater management in which recovery is always relatively limited (20% of N and P mass flows). Using an adapted framework, including an influent generator, alternative scenarios can be assessed, showing that more benefit would be reached by recovering fertilizers and energy from undiluted streams.[111,119,120]

Cost analysis models also deserve more attention. Whereas energy cost is generally well known, the market for new valuable products like struvite or polymers can be highly dependent on the local situation and regulation, making the approach more speculative and uncertain for such products.[121] The cost saving is generally considered whereas the benefit of product sale can be considered as an option. A local use or dedicated market is generally encouraged. Actually, water reclamation remains the main driver in cost analysis.[120]

Finally, recent papers describe the feasibility of coupling DM–LCA with multi-objective optimization (MOO).[112,122] The combined frameworks (DM–LCA–MOO) can be applied with three objectives: effluent quality index (EQI), operational cost index (OCI) and environmental impacts quantified through life cycle impact assessment (LCIA). Given the contradictory nature of objectives, Pareto fronts are generated through simulation, which can help decision making for selecting some recovery scenarios and operational conditions. The main challenges and research points of these approaches are related to uncertainty evaluation, sizing choice, dynamic aspects to be considered and system boundary definition.

4 Conclusions

• Despite being a simplification of reality, ASMs remain state-of-the-art for modelling conventional WWTP processes and can even be used to describe a significant part of the resource (energy, nutrients, and other products) recovery options.

• Extensions to 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 into process behaviours.

• A good resource recovery model should be able to predict product specifications, similar to 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 the life cycle, product quality and techno-economical aspects as additional important criteria associated with product formation.

Conflicts of interest

There are no conflicts to declare.

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