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Modelling demand response with process models and energy systems models: potential applications for wastewater treatment within the energy-water nexus

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Abstract

A promising tool to achieve more flexibility within power systems is demand response (DR). End users in many strands of industry have been subject to research regarding the opportunities for implementing DR programmes. We review recent DR modelling approaches in the realm of energy systems models and industrial process models. We find that existing models over- or underestimate the available DR potential from an industrial end user for two main reasons. First, the interaction between power system operation and industrial process operation caused by DR is not taken into account. Second, models abstract from critical physical process constraints affecting the DR potential. To illustrate this, we discuss the wastewater treatment process as one industrial end user within the energy-water nexus, for which the lack of suitable modelling tools is affecting the accurate assessment of the DR potential. Case studies indicate the potential for wastewater treatment plants to provide DR, but no study acknowledges the endogeneity of energy prices which arises from a large-scale utilisation of DR. Therefore, we propose an integrated modelling approach, combining energy system optimisation with the level of operational detail in process simulation models. This will yield a higher level of accuracy regarding the assessment of DR potential from a specific process, such as wastewater treatment.

Keywords: Energy-water nexus, demand response, industrial end users, wastewater treatment, flexibility, energy system, modelling

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1. Introduction

With increasing power generation from renewable energy sources (RES), electricity supply becomes increasingly variable. This necessitates more flexible energy demand sources, which can adapt to the variability in supply by providing Demand Response (DR). DR can be defined as "changes in electric use by demand-side resources from their normal consumption patterns in response to changes in the price of electricity, or to incentive payments designed to induce lower electricity use at times of high wholesale market prices or when system reliability is jeopardized."(Lee et al., 2013). The implementation of DR programmes reduces peak demand, such that the output from expensive and carbon-intensive peak units is decreased (Nolan and O'Malley, 2015). Consequently, it can help reduce the risk of power outages, defer capacity investments, improve the reliability of the system and is likely to reduce electricity costs for energy consumers (Kim and Shcherbakova, 2011). Research has looked at the DR potential of heating, cooling and transport extensively, but comprehensive assessment of the DR potential within the energy-water nexus is still very limited.

In general, the energy-water nexus (sometimes also the energy-water-food nexus or the energy-water-land nexus) refers to all processes which represent linkages between the water system and the energy sector, and the trade-off of both resources. Water is required for energy production (water for energy), energy is required for water services (energy for water), and both resources have close interconnections in production and consumption of products. Against the background of climate change, increasing global energy demand and increasing water scarcity (Rodriguez et al., 2013), research on the energy-water nexus gains more and more interest. The connections between the energy sector and the water sectors were first recognised in the early 2000's, for example with a focus on India (Malik, 2002) or California, US (Lofman et al., 2002). Since then, the number of publications on the energy-water nexus has increased significantly, from 8 publications in 2010, to 131 publications in 2018 (SCOPUS, 2019). The OECD acknowledges that "efficient management of the [land-energy-water] nexus resources needs to take into account the direct and indirect effects of changes in the demand and supply of the various resources on the whole biophysical and economic systems, as this is the only means to avoid negative side effects and to create synergies" (OECD, 2017).

Wastewater treatment is an important example of an electricity-intensive industrial process with DR potential within the energy-water nexus. Electricity costs generally account for the highest share of operating costs in medium and large-scale wastewater treatment plants (WWTP). Depending on the treatment level and plant size, estimated electricity costs can range from 2 to 60 percent of total operating costs. In countries with well-developed water distribution and treatment systems, the wastewater treatment sector can be a significant electricity consumer, accounting for about 3 percent of total electricity consumption of a country per year (Gude, 2015).

Several case studies have found that energy-consuming processes within WWTPs, such as pumping or aeration, allow for flexible operation. This potential flexibility, coupled with significant levels of total energy consumption, makes the wastewater treatment sector an interesting potential provider of DR from a power system perspective. However, there is no study which investigates the DR potential of the wastewater treatment sector and its economic and environmental effects on the power system and WWTP operation likewise.

In this paper, we investigate whether this is caused by a modelling gap among existing DR models. Therefore, we summarise published literature on DR modelling within energy system models and industrial process models. We find that the interaction between the power system and industrial process caused by DR is not well accounted for in either of these models. In order to illustrate this, we examine wastewater treatment as one particular end user process in detail. We point out that only a few publications look into DR with a WWTP simulation model, although several case studies indicate that there is significant potential for flexibility within WWTP operation. Case studies have analysed the potential for flexibility in wastewater pumping, intermittent aeration, using built-in redundancy for delaying treatment and sludge processing. The purpose of this paper is to demonstrate that the lack of modelling tools in the DR literature leads to an underutilisation of readily available demand flexibility in industrial processes, one example for this being wastewater treatment. In order to fill this gap, a novel integrated energy-water system model is required to capture these flexibility options in a WWTP process model in connection with the power system. In contrast to previous reviews of DR models, our focus on the energy-water nexus offers a novel perspective on existing DR literature.

The paper is structured as follows. Section 2 summarises the literature on existing DR models. We distinguish between energy system models, industrial process models and WWTP models. Since this paper focuses on the DR potential of wastewater treatment for the power system, we briefly describe energy costs in the water sector in section 3.1, before we describe the flexibility potentials within the wastewater treatment process in section 3.2. We discuss the current modelling approaches for DR in section 4 and propose the development of a combined system-process model for the analysis of the DR potential from WWTPs. We conclude in section 5.

2. DR models

DR is one of many sources of flexibility within energy systems that can be harnessed. We define DR as any change of the usual electricity demand pattern in response to a price signal from the electricity supplier. The individual characteristics of an end-user process, such as intertemporal interdependency of processes, required timing precision in a process, or the energy infrastructure on site (i.e. electricity meters and sensors) determine its DR potential and influence the decision for a DR strategy. One possible option is load shedding, where the electricity use is reduced during peak hours without a change of the consumption pattern during the rest of the time (Albadi and El-Saadany, 2008). Another option is to shift electricity demand from peak to off-peak periods (Albadi and El-Saadany, 2008), while not reducing the overall consumption. Load shifting is particularly beneficial for processes with a certain degree of inertia or storage capabilities (Palensky and Dietrich, 2011). On-site electricity generation increases flexibility in terms of electricity demand from the grid as well. However, we do not view this as DR according to our definition, since producing electricity on-site does not lead to a change in consumption pattern, but rather to a change in electricity supply sources.

The literature on DR modelling is extensive and comprehensive reviews on DR models have been previously undertaken. For example, Boßmann and Eser (2016) analyse 117 DR models and cluster them in terms of pricing schemes, electricity systems, specific end-uses and control-strategies. They find that existing DR models are highly heterogeneous and the field lacks a body of standard models. One major insight from their analysis is that the residential sector is in the focus of many models, while industrial end-users are underrepresented. They also find that a majority of models deal with system performance, while little attention is paid to control strategies. Deng et al. (2015) also perform a short summary of DR models and categorise the existing literature in terms of the mathematical modelling approach. The most used approaches are convex optimisation, game theory and dynamic programming. Other modelling approaches include Markov decision processes, stochastic programming and particle swarm optimisation. The review by Wang et al. (2017a) focuses on integrated DR in multi-energy systems. They focus on DR provision by processes in between the energy sectors of electricity, thermal energy and natural gas. It shows that research on the DR modelling of heat pumps and power-to-gas technologies is extensive. However, they point out that most studies develop a detail model of these devices, while neglecting the energy system effects. Zhang and Grossmann (2016) review scheduling models for industrial processes in order to determine operational flexibility as a precondition to provide DR. Most of those models focus on continuous processes, such as cryogenic air separation, aluminium and cement production, the chlor-alkali process, flour and pulp production, machining and steel production. The authors find that the models reviewed either apply a network structure with material handling constraints or base the modelling on operating modes, where the process can only operate in one of a number of predefined states.

The present review represents a significant advance on the literature by considering and identifying the differences between energy system models and industrial process models, particularly in their treatment of DR. Furthermore, we provide detailed analysis of the DR potential of the wastewater treatment process as a cogent example of an end user process, within the energy-water nexus, that has received limited attention in the literature to date. This work shows that a sector-integrating energy system model which can represent the wastewater treatment process as well as the power system dynamics does not yet exist. None of the reviews addresses this gap among existing DR models with respect to the energy-water nexus.

2.1. Energy system models

We review publications between 2001 and 2019 which incorporate DR within energy system models. We focus on methodology rather than results for the purposes of this analysis. Most of the models are economic dispatch (ED) or unit commitment (UC) models with a cost minimisation approach. We also find some capacity planning models accounting for DR, as well as game theoretical models.

ED models aim to minimise the operating cost of the whole energy system by determining the optimal power output and fuel consumption of each generator at each point in time (Zhu, 2015). Other model outputs depend on the level of detail in the model. Most models incorporate the level of emissions caused by fuel use, such that environmental effects are also in the scope of analysis. The optimisation is subject to constraints including the energy demand, technological constraints of generating units, availability of resources and fuels or regulatory constraints. Many models also incorporate the level of emissions caused by fuel use, such that environmental effects are also in the scope of analysis. A simple formulation of an ED model can be found in appendix 1.

UC models also determine the optimal output of each generator at each time step, but additionally consider that generators can be turned on or off dynamically. This means that not necessarily all available generators in the system produce electricity all the time. The decision to engage a generator depends on the trade-off between the costs for that generator of providing energy and the costs of switching it off. This makes the UC problem more complex than an ED, since the model is optimised over the whole optimisation period at once. The mathematical structure of the problem changes from a linear optimisation problem in the case of ED to a mixed integer linear programme for UC due to the

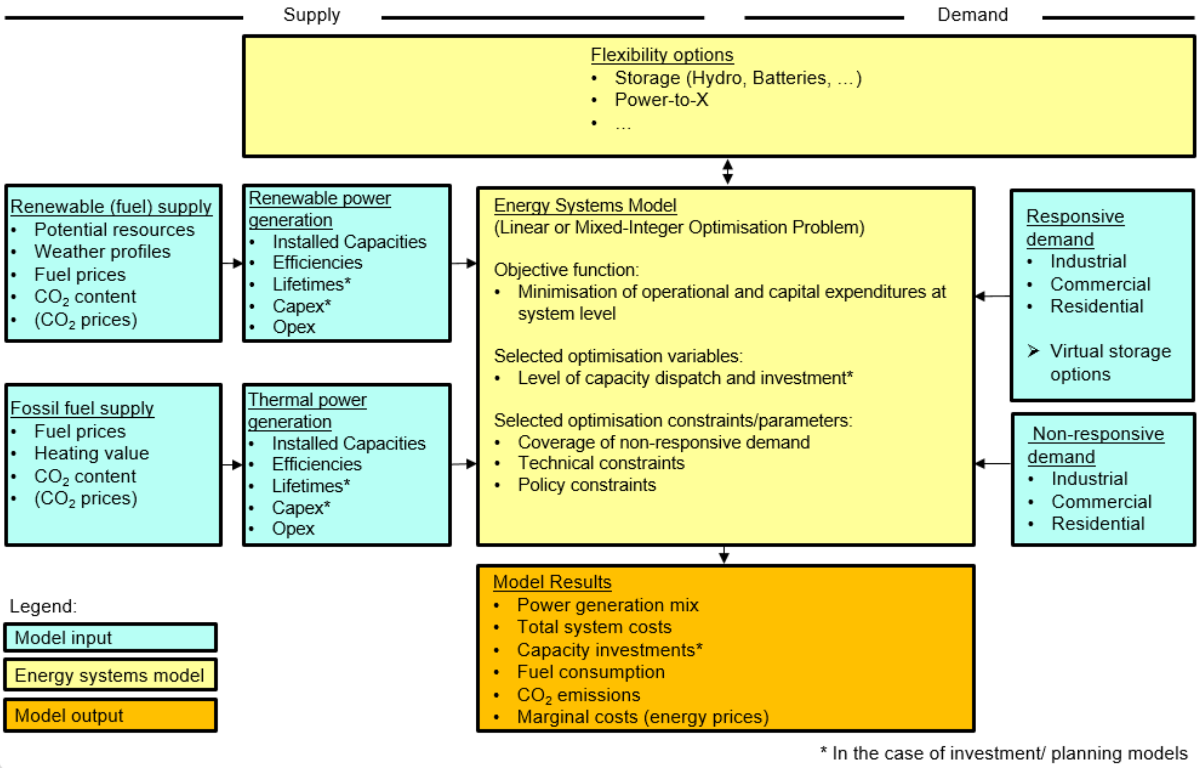

Figure 1: Schematic energy system model

binary decision whether to switch generators on or off. An example of a simple UC is given in appendix 1.

Additionally, stochastic UC can be used for representing uncertainties related to renewable energy generation (Papavasiliou and Oren, 2012) and studying their effect on the participation in DR programmes. Figure 1 depicts the general structure of a traditional energy system model in the form of an ED or UC model.

Game theoretic models of DR do not have a single objective function which is optimised for the whole energy system, but acknowledge the presence of multiple players with individual objectives within the system. The outcome of the optimisation depends on the structure of the game, e.g. the order in which players choose their strategies and which information is available to them. Therefore, these models can account for strategic behaviour among players, as well as for information asymmetries.

Subsequently, we review publications with respect to two questions: First, is the DR resource modelled in a generic way or is the DR resource specified as a particular end-user? Second, does the model integrate different energy sectors, such as electricity (E), heating (H), cooling (C), power-to-gas (P2G) and transport (T)? These criteria will show whether there is a modelling gap among system models for integrated energy system approaches with end-user specific DR. We also categorise the energy system models into UC, ED, Capacity Planning (CP) and Game Theory (GT) models. Furthermore, we describe the focus of the publication, the methodology used and the case studies for which the model was tested. A summary of the reviewed literature in terms of these criteria is given in Table 1.

Table 1: Energy system models incorporating DR ...

Publication	**Focus**	**DR modelling**	**Energy sectors**	**Model type**	**Methodology**	**Case study**
		Generic DR				
Keane et al. (2011)	Wind penetration	Load shifting units as energy storage	E	UC	deterministic MILP (WILMAR)	Ireland
Dietrich et al. (2012)	Wind penetration	Centrally chosen DR and elastic demand	E	UC	deterministic MILP	Gran Canaria
Wang and Li (2015)	Wind penetration	DR aggregators	E	UC	two-stage stochastic program	PNJM 5-bus system, IEEE 118-bus system
Kwag and Kim (2012)	DR constraints	Virtual generations units, self-provided customer information	E	UC	stochastic DR participation, MILP	6-bus test system
Papavasiliou and Oren (2012)	Decentralisation	Decentralized approach: bid valuations and DR in objective function; centralized approach: DR determined by system operator; Coupling: deferrable loads coordinate with renewable suppliers	E	UC	two-stage stochastic MILP	Model of the Western Electricity Coordinating Council (WECC)
Ikeda and Ogimoto (2013)	Energy storage	generic DR resource	E	UC	stochastic model	Power systems in Tokyo and Tohoku
Liu and Tomsovic (2014)	Demand bidding	Duplex bids in energy market and reserve market	E	UC, ED	two-stage stochastic MILP	IEEE Reliability Test System
Behrangrad et al. (2012)	Air conditioning	DR aggregator	E, C	UC, ED	stochastic real-time dispatch	32-unit test system IEEE RTS 1996
Wang et al. (2013)	Spinning reserve	Aggregation into virtual power plants	E	ED	non-linear program with stochastic loads	Modified version of the IEEE 14-bus transmission system
Moura and de Almeida (2010)	multiple objectives	Shift of demand curve	E	ED	LP	Portugal
Abdi et al. (2016)	Non-linear responsive loads	Total hourly demand elasticity	E	ED	non-linear deterministic model	ten units test system
Xu et al. (2017)	Wind penetration	elastic loads and dynamic incentive mechanism	E	ED	stochastic MILP	IEEE 24-bus Reliability Test System
Tan et al. (2014)	Energy storage	generic DR	E	ED	non-linear two-stage model	IEEE36 node 10 machine systems
Choi and Thomas (2012)	Environmental policies	Demand elasticities	E	CP	deterministic MILP	Georgia, US
De Jonghe et al. (2012)	Wind penetration	elastic demand functions that account for load shifts among hours	E	CP	Static, single node LP, with DR added as complementarity or quadratic program, or Piece-wise Integration algorithm	Denmark
Koltsaklis et al. (2015)	Capacity development	Reference demand and Monte Carlo Simulation	E	CP	Multi-regional, multi-period linear MILP	Greek power system

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Table 1: Energy system models incorporating DR . . . (cont.)

Publication	Focus	DR modelling	Energy sectors	Model type	Methodology	Case study
		Specific DR				
Zhong et al. (2015)	Industrial consumers	Load adjustment costs, individual load profiles	E	UC	deterministic MILP	IEEE 30-bus system and a real-world system in China
Paulus and Borggrefe (2011)	Energy-intensive industries	Technical constraints for five industrial processes	E	CP	stochastic LP (DIME)	Germany
Mohsenian-Rad et al. (2010)	Autonomous DSM between end-users	Household appliances connected to automatic ECS	E	GT	linear and convex programming	Benchmark system with 10 consumers
Lynch et al. (2019)	Capacity markets	DR aggregator and heat demand derived from building model	E, H	GT	Mixed Complementarity Problems	Irish test system with 6 generators
Shao et al. (2017)	Integration of heat and electricity	DR aggregator with connected heating system	E, H	ED, GT	bilevel program, LP with piecewise-linear demand functions	30-bus test system
Linna et al. (2018)	Diversified storage options	Energy hubs with P2G and heat pumps	E, H, P2G	ED, GT	bilevel approach: nonlinear and quadratic program	4-bus multi-energy system, revised IEEE 118-bus power system and a 20-bus Belgian gas system
Zhao et al. (2018)	Industrial parks	Model of integrated DR, composed of separate models for Electricity DR and heating and cooling DR	E, C, H, gas	GT	bilevel stochastic MILP	Industrial park in China, with 13 lower-level factories and one multi-energy operator
Hedegaard et al. (2012)	Heat pumps	Black-box heat pumps with heat balance equation, with heat accumulation tanks or/and passive heat storage of building	E, H	ED	deterministic MILP (EnergyPLAN)	Danish energy system in 2020
Papaefthymiou et al. (2012)	Heat-pumps	Detailed dynamic thermal simulation model	E, H	ED	stochastic MILP (PowerFys)	German electricity system
Lund and Kempton (2008)	EVs	Aggregated vehicle fleet and operational constraints	E, H, T	ED	deterministic MILP (EnergyPLAN)	Denmark
Soares et al. (2017)	Uncertainty in PV, EV, wind, market prices	DR aggregator, incentive payment for load reduction and EV fleet with samples of driving patterns	E, T	ED	two-stage stochastic MILP	system with 201 buses from Zaragoza, Spain
Fehrenbach et al. (2014)	Residential heating	Thermal storage in buildings and heat pumps via model constraints	E, H	CP	partial-equilibrium LP (TIMES)	Germany
Zugno et al. (2013)	Electricity retailers and consumers	Three-state state space model for heating dynamics and storage	E, H	UC, GT	bilevel programme and single-level MILP	small test system with 3 consumers

Generic and end-user specific DR

Most studies which investigate DR within an energy system model do not specify the type of end-user providing DR, but rather incorporate a generic DR resource. For some models, this means that DR is modelled as a portion of the total system demand, which can be shifted from peak hours to off-peak hours. A mathematical example for this can be found in appendix 2. For example, this is the case for Moura and de Almeida (2010), who develop an ED model with multiple objectives. In order to incorporate DR into their capacity planning model for the Greek power system, Koltsaklis et al. (2015) start with a reference demand function and use Monte Carlo simulation to derive a flexible demand function.

Another way of modelling DR generically is to account for demand elasticity, either in the total system demand or for different individual consumers. For example, Abdi et al. (2016) develop a non-linear scheduling approach for responsive loads, where demand elasticities are defined for every hour. Xu et al. (2017) also present a model of elastic load functions, combined with a dynamic incentive mechanism to foster DR participation. De Jonghe et al. (2012) specifically include cross-price elasticities into the elastic demand functions for individual consumers to account for load shifts among hours. Dietrich et al. (2012) investigate the contrast of modelling DR by means of demand elasticities, taking into account consumer preferences, with a scenario where DR is modelled as a DR resource that the system operator can control directly.

Finally, a common way of modelling DR is the representation via DR aggregators or virtual power plants. Kwag and Kim (2012) model DR resources as virtual power generating units and impose operational constraints on them based on self-provided customer information. Keane et al. (2011) model load shifting units similarly to energy storage units. They argue that the purpose of shifting demand in time is the same for energy storages and DR resources. An example for DR aggregators is given by Wang and Li (2015). They model five DR aggregators with heterogeneous cost structures and explore how they affect each other with and without transmission constraints.

The advantage of these models is that by modelling DR in a generic way, the analysis can be focused on the system effects of DR. For the research questions in these models, it is irrelevant how DR is provided. However, there is a risk of over- or under-evaluating the available DR potential by not taking into account the specific characteristics of an end-user providing DR.

In contrast, system models which incorporate specific DR resources are able to represent the DR potential more accurately. Most commonly, those models introduce a homogeneous population of the respective resource and impose constraints on their operation. One early model which focuses on DR from electric vehicles (EVs) is developed by Lund and Kempton (2008). DR is provided by an aggregated vehicle fleet, and the optimisation is, inter alia, constrained by the total transportation demand, distribution of transportation demand, power capacity of EV grid connection, maximum share of EVs during peak demand, battery efficiency and capacity and the share of parked cars. Soares et al. (2017) model an EV fleet with similar constraints and enhance the model by adding samples of typical driving patterns.

Heat pumps are also often in the focus of DR system models and represented in a similar manner. Hedegaard et al. (2012) model a heat pump population constrained by a heat balance equation. Flexibility comes from heat accumulation tanks or/and passive heat storage of the respective building. Similarly, Fehrenbach et al. (2014) include thermal storage in buildings and heat pumps via operational constraints imposed on the optimisation problem.

Paulus and Borggrefe (2011) focus on the DR potential from energy-intensive industries. In their capacity planning model, they investigate potential DR provision of the chlor-alkali process, mechanical wood and pulp production, the aluminum electrolysis, electric arc furnace (to produce steel) and cement mills for the German electricity system. For their analysis, they use the Dispatch and Investment Model for Electricity Markets in Europe (DIME), which is a linear optimisation model that minimises total system costs. Within this framework, Paulus and Borggrefe model DR resources with a potential for load shedding similarly to power plants and processes with the potential for load shifting as energy storage units. Technical restrictions which ensure minimal disruption of the production process and cost parameters define the extent to which the DR resources are developed and exploited in the system. Zhong et al. (2015) also focus on DR from industrial consumers. They introduce the concept of load adjustment costs, expressing the willingness of consumers to change their load pattern. Thereby, the operational constraints of the industrial process are implicitly included in the resulting load profiles of the consumer, rather than directly in the optimisation problem.

Other DR system models address end-user specific DR with a two-stage optimisation approach. For example, Zugno et al. (2013) model the relationship between electricity retailers and consumers as a Stackelberg game with a dynamic pricing scheme. They formulate the optimisation problem as a bi-level programme and model the thermal storage and heating dynamics in buildings via a three-state, discrete-time state space model. Papaefthymiou et al. (2012) couple a detailed dynamic thermal simulation model of specified reference buildings with an electricity system model. In a first step, the thermal building model allows for the assessment of the operational restrictions of heat pumps within the building. Subsequently, the system model incorporates the building stock's thermal behaviour as a form of energy storage in an electricity market. A mixed-integer stochastic optimization model called PowerFys is used for modelling the day-ahead and intra-day electricity markets with an hourly resolution, with particular emphasis on wind forecast uncertainty.

Since these models account for specific characteristics of the respective end-user, the flexibility and the quantity of DR provision are represented more accurately. This makes them more suitable for the analysis of the effects of DR on both the energy system and the DR provider than models with generic DR. By including the operational constraints for the end-user into a single-stage optimisation problem, the system operator is assumed to be able to choose the optimal operation and DR provision of the end-user. The analysis yields the optimal technically available DR potential, accounting for the mutual influence of system operation and end-user operation. However, most models implement a homogeneous population of one end-user type and impose operational constraints which do not account for the inner processes of the DR resource. This can mean that important operational constraints are neglected, which can lead to an incorrect estimation of the DR potential. In contrast, game-theoretic approaches with specific end-users acknowledge strategic behaviour and informational asymmetries between DR providers and system operators. The resulting two-stage optimisation problem can better account for operational detail within the end-user process, but the solution is often sub-optimal, either for the end-user or for the power system. So far, detailed models like this only exist for the thermal storage capacity of buildings, where heating dynamics are taken into account.

Integrated energy system models and multi-sector models

Most DR models reviewed focus on analysing DR within the electricity system, and do not account for other energy sectors. Among multi-sector DR models, one can distinguish between integrated energy models and models of interlinked energy sectors. The majority of these DR system models focus on the linkages between electricity and either heating or transport.

Integrated energy system models incorporate all relevant energy sectors into one optimisation problem. The advantage of this approach is that the solution generally yields the global optimum for the operation of the combined system. On the downside, the resulting multi-sector energy models can be very complex, depending on the size of the system and the level of detail. Therefore, it is generally not expedient to include a high level of detail into the modelling of individual technologies.

Lund and Kempton (2008) use a general energy system analysis tool called EnergyPLAN to investigate energy sector integration within the Danish energy system. EnergyPLAN is a deterministic input-output model and integrates the electricity, transport, industry and district heating sectors. It incorporates data on technology capacities in the system, conversion efficiencies between different energy sources, energy demands, fuel costs and CO2 costs. The model outputs comprise energy balances, energy supply, fuel consumption, electricity imports/exports, CO2 emissions, and costs. Within this framework, Lund and Kempton investigate the linkages between the electricity sector and the transport sector. They use the model to analyse the flexibility potential of EVs and the potential for the "vehicle-to-grid" technology as an energy storage option. Thereby, they also investigate whether demand flexibility in the transport sector can help reduce the excess of wind energy.

Soares et al. (2017) integrate the electricity and transport sectors in their model by taking into account an EV fleet with system-wide operational constraints for charging and discharging. However, other constraints on EV utilisation are not introduced (in contrast to Lund and Kempton (2008)). Instead, different samples of driving patterns, using departure times and locations as stochastic variables, are used. Hedegaard et al. (2012) also use EnergyPLAN for their analysis of DR within the electricity sector and the heating sector. They explore the utilisation of compression heat pumps and heat storage devices to integrate more wind energy into the power system.

Another single-stage optimisation model which investigates DR from the heating sector in an integrated energy system is Fehrenbach et al. (2014). They use the TIMES (The Integrated MARKAL-EFOM System) model, which is a widely used energy system optimisation tool and combines a-technical engineering and an economic perspective. It uses linear-programming to produce a least-cost solution for the energy system over medium to long-term time horizons (Loulou et al., 2005). Fehrenbach et al. (2014) use TIMES for modelling the electricity and residential heat supply in Germany and to determine capacity developments and dispatch of electricity and residential heat generation technologies until 2050.

Another approach is the subsequent optimisation of two energy sectors. This can be beneficial when the level of complexity of one energy sector model is particularly high, such that an integrated optimisation approach would be computationally intensive to solve. It is also suitable for models where the operation of one energy sector is optimised depending on the operation of the other, such as in game-theoretic approaches. However, vice-versa effects of DR cannot be studied in this context, because the operation of one energy sector is assumed exogenous for the optimisation of the other energy sector operation.

One example for a model of interlinked energy sectors is Papaefthymiou et al. (2012). They couple a detailed thermal model of six reference buildings with a high-level electricity market model. Different scenarios of heat pump operation (business-as-usual and demand shifting) are determined within the buildings simulation model and incorporated into the electricity model afterwards.

Zugno et al. (2013) use a three-state, discrete-time state space model for the heating dynamics based on Halvgaard et al. (2012) to model electricity consumer decisions. The model considers indoor temperature, floor temperature and the temperature inside a water tank directly connected to a heat pump. Outdoor temperature is treated as a stochastic exogenous parameter and solar irradiation is neglected. Electricity retailer decisions are then driven by profit maximisation. Although this bi-level program is the starting point of the model, an integrated MILP is later derived such that the final optimisation problem is solved simultaneously for both players.

In summary, the review shows that multi-sector DR is well explored for linkages between electricity, transport and heating. However, we did not find any DR system models that address potential sources of DR within the energy-water nexus.

2.2. Industrial process models

The focus of our review now turns to DR within industrial process models. In contrast to energy system models, industrial process models focus on a process, device or application of a particular end user. Usually, these models take energy prices as an input and evaluate DR potential by comparing different electricity tariff schemes. In some cases, these price patterns are derived from running an electricity market simulation prior to the process model.

Modelling approaches for industrial processes can be either model-based or data-driven. One model-based approach involves the detailed description of the system's performance, e.g. its thermodynamics and kinetics (Mitra et al., 2012). This requires the formulation of heat and mass balances for each process module. The resulting simulation models often consist of a set of non-linear differential equations that are based on fundamental physical principles. Simulation models are suitable for analysing the effects of different set-points for controllable parameters within the system (so-called controllers) on the process performance.

However, following this approach can make a model extremely complex due to its non-linearity and its size, rendering it difficult to solve for longer time horizons. Therefore, process optimisation models focus on the electricity demand of the process and abstract from the physical details by using LP or MILP approaches. The objective of these models is to find an optimal process schedule given the technical constraints of the process and cost parameters. Despite their wide application, there is a risk that these models over- or underestimate the DR potential by neglecting the physical details of the process.

Finally, data-driven approaches use regression models to establish a meaningful relationship between input and output data of the respective process, for example by using machine learning techniques. They require greater amounts of data compared to simulation models, but can be advantageous when details of the process operations are unknown. A schematic industrial process model is given in figure 2.

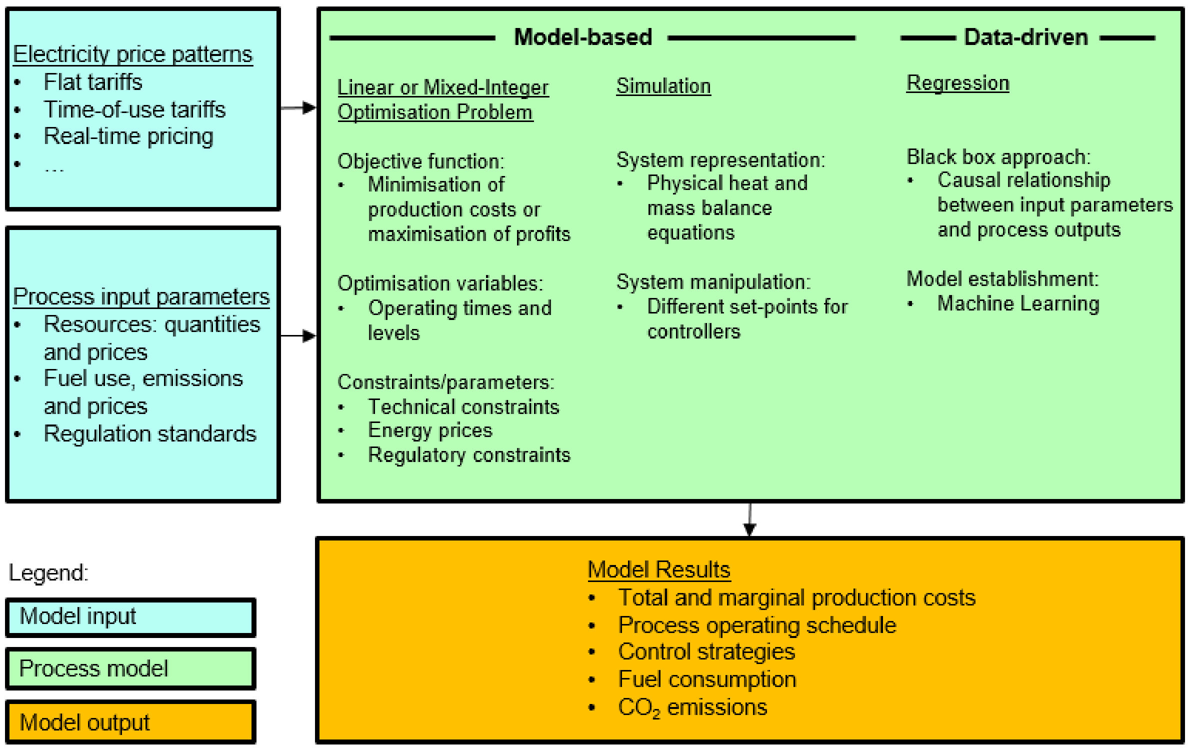

Figure 2: Schematic industrial process model

Several process models deal with the DR potential from industrial processes. For the selection of relevant literature, we focused on the type of industrial process studied and the applied methodology. Table 2 gives an overview of the reviewed industrial process models analysing DR.

Table 2: Industrial process models incorporating DR

Publication	Industrial process	Methodology
Zhang et al. (2016)	Industrial loads	Model predictive control
Hindi et al. (2011)	Industrial process	Model predictive control
Ding and Hong (2013)	Steel plant	State task network (STN)
Ding et al. (2014)	Industrial consumers	STN and MILP
Reka and Ramesh (2016)	Refinery industrial plant	Resource-task network processing model
Desta et al. (2018)	Soft/hard biscuit production	Finite state machine, local search heuristic
Mohagheghi and Raji (2014)	Vehicle cockpit manufacturing	Fuzzy logic
Rodríguez-García et al. (2016)	Industrial consumers	Dynamic simulation
Ashok (2006)	Steel plants	Integer programming
Abdulaal et al. (2017)	Industrial loads: multistage chiller system, EV charging and discharging for building's demand support (V2B)	Quadratic, stochastic, and evolutionary programming with multi-objective and continuous simulation
Sianaki et al. (2018)	Industrial consumers	Linear programming
Schoepf et al. (2018)	Paper industry	Linear programming
Seier and Schebek (2017)	WWTP	Linear programming
Middelberg et al. (2009)	Colliery process	Binary integer programming
Wang et al. (2017b)	Chlor-alkali plant	Convex optimisation
Mitra et al. (2012)	Air-separation process	Deterministic MILP
Helin et al. (2017)	Pulp an paper mill	MILP
Ramin et al. (2018)	Metal casting plant	MILP
Jiang et al. (2018)	Industrial consumers	LP with piecewise-linear heat and electricity demand

One possible and commonly applied control approach in industrial process models is Model Predictive Control (MPC). It uses state variables and a detailed mathematical system model in order to predict system outcomes based on stochastic system disturbances (Lauro et al., 2015). Usually, the computational complexity of MPC models is high, but in contrast to data-driven approaches, they do not have large data requirements from specific buildings (Lauro et al., 2015).

Zhang et al. (2016) recognise that many industrial processes can technically provide fast DR, but most of them can only vary electricity demand discretely in the form of certain Megawatts at a time. However, providing fast DR can require a more granular change in power. In order to overcome this, the authors propose a process model which incorporates on-site energy storage. As a case study, the authors choose mills in a cement plant, which can be switched on and off very rapidly. An MPC coordinates a large discrete power change provided by the industrial process and a small continuous power change provided by the energy storage, such that the total power change accurately follows the DR signal. The MPC approach combines a stochastic model for inputs, e.g. a price signal, with a short-term optimisation of the connected processes. In the model, DR is achieved by incorporating the satisfaction of the DR signal along with the number of switching actions in the objective function of the optimisation model. The results demonstrate that the MPC regulates both the industrial loads and the energy storage effectively to provide fast and high-quality DR.

Ashok (2006) develops a load model for small steel plants in India under a time-of-use (TOU) tariff regime. A TOU pricing scheme consists of different tariff periods throughout the day, for example peak and off-peak periods, with a higher charge during peak periods (Samad and Kiliccote, 2012). The model is coupled with an optimisation formulation utilising integer programming for minimising the total electricity cost satisfying production, process flow and storage constraints. The author claims that it can also be applied to other batch-type processes. Middelberg et al. (2009) explore optimal control strategies of the colliery process and conduct a case study for a colliery in South Africa. The control strategy emerges from minimising the total electricity costs of the process, with a binary decision variable for every module of the process. They discretise the time horizon of the optimisation window, which turns the scheduling problem into an integer programme.

Mitra et al. (2012) develop a discrete-time, deterministic mixed integer linear model for scheduling power-intensive continuous processes. The objective function is composed of the production cost, inventory cost and transition cost of the process. This is minimised for every hour with an emphasis on the operational transitions, which arise from switching the operating modes of the process modules. They show that certain logic constraints limit the flexibility in control severely. Given an hourly electricity price pattern, they conduct a case study on air-separation plants and cement plants and demonstrate that their model yields practical schedules, while minimising the number of changeovers.

Ding and Hong (2013) provide a process model for industrial consumers which can incorporate on-site electricity generation, e.g. by solar panels, wind turbines or waste heat recovery, and energy storage. The mixed integer linear model is based on a state task network (STN) approach, which divides tasks into non-schedulable and schedulable. Hence, only schedulable tasks can be used to provide DR, because they can be run in multiple operating modes, with varying production rates and electricity demand. This structure yields a relatively straight-forward framework to model any industrial process with a focus on DR. Ding and Hong (2013) demonstrate the model structure with the help of a case study for steel manufacturing facilities. However, they do not provide any results on the scope of DR in this case study nor specify the required DR algorithms and strategies according to which the tasks should be scheduled.

In another study, Ding et al. (2014) apply the same model to the industrial oxygenating generation, which is part of many industrial processes like steel and glass manufacturing or wastewater treatment. DR decisions are based on day-ahead hourly electricity prices. The optimisation yields a process schedule where energy demand is shifted from peak to off-peak periods, which results in a reduction of total energy costs.

Reka and Ramesh (2016) use a similar approach called resource-task network processing modelling. They also distinguish between schedulable and non-schedulable tasks within the process, but pay special attention to the resources consumed in every task. They use stochastic optimisation with discrete time steps. The proposed DR algorithm aims to minimise the total process costs. The model is tested with a case study for an oil refinery with on-site electricity co-generation facilities. The most energy-intensive refinery sub-processes are desalination, hydro-treatment and crude oil distillation. Findings suggest that employing DR strategies for schedulable tasks yields a shift in energy demand from peak to non-peak periods.

Rodríguez-García et al. (2016) introduce a model for industrial customers to perform a cost-benefit analysis of the implementation of DR strategies. In contrast to most other (prescriptive) models that we found, this is a dynamic simulation model, which relies on the identification of typical load curves by an energy audit. The decision criterion for whether a process should participate in DR is the difference between the net amount of money that the industrial customer receives due to the participation in the reserve energy market, and the expected benefit for the customer. The authors make the model available to industrial customers as an online tool and show an application for a German paper factory. Although they claim that the model has been validated in four real industrial sites from different parts of Europe, it does not sufficiently account for the interdependence of sub-processes and therefore yields a skewed picture of the economic DR potential.

Wang et al. (2017b) conduct a case study on DR from a grid-connected chlor-alkali plant with an integrated on-site energy recovery system. They develop a communication and incentive scheme that incorporates day-ahead process scheduling according to the electricity contract, as well as real-time DR. Total operating and environmental costs through producing, purchasing and selling electricity are minimised while meeting production requirements. The results show that the average electricity costs are lowest with an energy contract based on demand responsive behaviour.

Seier and Schebek (2017) develop a linear optimisation model of a WWTP that focuses on biogas usage to cover electricity demand. They assess the effects of load shifting by WWTPs in Germany on residual load smoothing. The residual load refers to the total power consumption minus the feed-in of renewable energies. The load shifting potential arises solely from a biogas storage option, which can be used to generate electricity on-site in a CHP plant. Seier and Schebek use a separate merit order simulation to model wholesale electricity prices, which are then fed into the WWTP optimisation.

The review of industrial process models shows that no model accounts for the vice-versa interaction with the power system when providing DR. Instead, models account for the electricity sector by using electricity price patterns as a model input. That means that the effects of industrial DR on the power system are out of the scope of these models. We only find one publication which specifically deals with DR from WWTPs (Seier and Schebek, 2017). However, the model represents WWTPs solely as biogas users or providers and neglects all other processes within a WWTP. In order to perform an analysis of the effects of DR provision on the whole process, a process simulation model can be more suitable.

2.3. WWTP models

Within end user process models, one example for a well-established process simulation model is the Activated Sludge Model 1 (ASM1), developed by Henze et al. (1987) to model municipal activated sludge plants. Activated sludge is the most common technology used in WWTPs with secondary treatment. The purpose of the process is the removal of biodegradable organic matter, nitrogenous compounds and suspended solids (Tchobanoglus et al., 2003). The core process includes the injection of air into the reactor tanks, which facilitates the growth and respiration of micro-organisms that are able to break down organic and nitrogenous matter in the wastewater (Aghajanzadeh et al., 2015). Figure 3 depicts the basic activated sludge process. It consists of a primary settling tank, an aerated tank in which the micro-organisms are kept in suspension, a sedimentation tank to separate liquids and solids by gravitation, and a recycle system which returns sludge back into the aerated tank (Tchobanoglus et al., 2003).

The ASM1 describes the biochemical processes within the aerated tank by eight processes

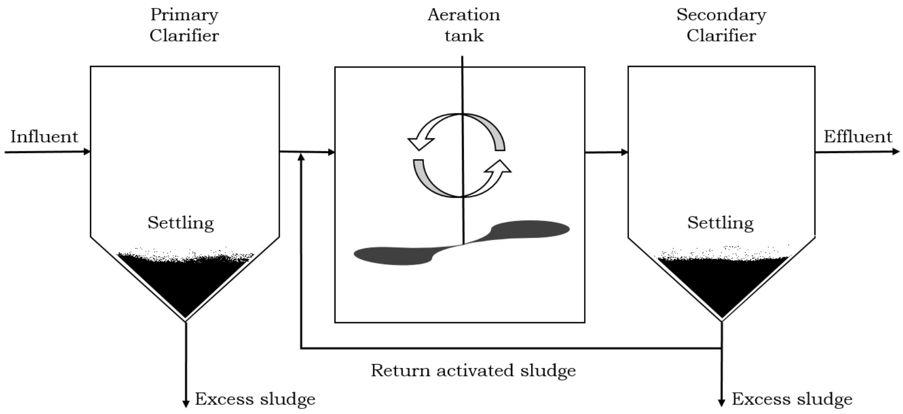

Figure 3: Basic activated sludge process

and 13 state variables (Jeppson, 1996). A reduced form of the model, without the description of the dynamics of alkalinity, is given in appendix C. For each step of the process, mass balance equations are established, which must be respected at any point in time. Since the first introduction of the ASM1 model, it has been updated and extended twice to account for initial shortcomings. The latest version, the ASM3 model, proposed by Gujer et al. (1999), corrects for a number of shortcomings of the ASM1 model, like inflexibility in settings for the external temperature, pH values, water toxicity, wastewater composition and the kinetics of bio degradation. Both ASM1 and ASM3 are used for WWTP design and for determining optimal process control strategies.

Based on these models and benchmark data, commercial WWTP simulators are available to model the whole WWTP process or specific sub-processes. These WWTP simulators often contain a pre-installed library of WWTP layouts. The process can easily be configured by connecting predefined unit blocks and modifying the model parameters. Examples of commercial modelling software are AQUASIM, BioWin WEST, EFOR, GPS-X, ICS, SIMBA#water, STOAT and Sumo. With the help of these simulation platforms and based on the ASM model family, a variety of WWTP models have been developed. They differ in plant layout and treatment technology and are often build to fit the characteristics of a real WWTP.

Other WWTP applications like the prediction of the influent load or the estimation of biomass activity and effluent quality use black-box or stochastic grey-box approaches (Gernaey et al., 2004). White-box models can also be complemented by Artificial intelligence (AI) methodologies, for example in the form of supervisory control systems (Gernaey et al., 2004). While white-box models can only evaluate scenarios based on existing process knowledge about the WWTP, AI methods can also extrapolate knowledge from experience, in order to enhance WWTP control (Gernaey et al., 2004).

WWTP models dedicated to minimising the energy costs of the process (particularly by optimising the aeration schedule) often employ a bio-kinetic model like the ASM1 in connection with an electricity tariff structure. For example, Póvoa et al. (2017) couple the ASM1 model with an energy pricing and a power consumption model to explore the cost efficiency of different control strategies. Energy prices are represented in three different ways: real energy pricing, weighted arithmetic mean energy pricing and arithmetic mean energy pricing. They find that modelling diurnal variations in energy prices instead of constant energy pricing enables the wastewater utility to optimise plant operation with respect to minimum energy consumption.

The WWTP model of Emami et al. (2018) deals with the effects of influent variations on energy costs for aeration and the related GHG emissions. A bio-kinetic model for the AS process is employed first to derive oxygen requirements based on the influent characteristics. Then, an aeration submodel determines the air requirements, which subsequently determines energy consumption and GHG emissions. A TOU tariff is used for the energy price structure. However, a shift of operation according to the TOU tariff is not considered. This is because the diurnal pattern of influent flow is inverse to the energy price structure, i.e. the maximum energy consumption occurs in peak hours and the minimum energy consumption in off-peak hours. Therefore, the authors conclude that shifting operation in time could result in non-compliance with the effluent standards.

Aymerich et al. (2015) model a WWTP based on the Benchmark Simulation Model 1 (BSM1) layout in SIMBA#. The BSM1 is a full-scale WWTP model which uses the ASM1 to describe the biokinetic processes within the aerated tank. The authors investigate the effect of different electricity tariff structures on the energy bill. They address three different tariffs: flat energy tariffs, TOU tariffs and a tiered rate, which increases when a certain threshold for the energy consumption is reached. Different control strategies and set points for the aeration process are studied. Their results show that using average energy prices instead of time-varying prices can lead to a biased selection of operating strategies, technologies and equipment.

Giberti et al. (2019) investigate the effects of electricity demand shedding in the aeration process on plant performance by means of a modified version of the BSM1 under different pollutant loading conditions. Their dual-layer settling model is capable of representing activated sludge settling when the aeration is turned off. Demand shedding is modelled by switching off the aeration in the last aerated tank for 1 hour, between 5pm and 6pm. This time interval is chosen due to a typical electricity demand peak at that time of day. However, electricity prices are not considered explicitly in this study, since it is focused on the effects of demand shedding on pollutant removal rather than energy costs. Results demonstrate the importance of modelling particulate settling within the aerated tank for evaluating the impact of DR on effluent quality accurately.

Recently, data-driven approaches have become more popular to investigate energy costs and saving potentials of WWTPs. For example, Asadi et al. (2017) use a data-mining approach based on input-output data to optimise the aeration process of a WWTP in Detroit, MI. The authors use a combination of the multi-adaptive regression spline (MARS), Artificial Neural Networks (ANN), Random Forest (RF) and K-nearest neighbor (k-NN) to construct the aeration model. The approach is data-intensive, as the training set for the algorithms contains 4368 data points and the testing set contains 2544 data points. The model minimises the dissolved oxygen (DO) concentration in the wastewater as a proxy for energy consumption for aeration.

Torregrossa et al. (2018) also use machine learning for modelling energy costs of WWTPs. Their data set contains energy consumption and intensity, energy prices, wastewater inflow mass and pollutant loads, pollutant loads at the outlet of the plant and plant sizes of 317 WWTPs using CAS technology, located in Northwestern Europe. They use NN and RF algorithms to generate regression models of energy costs. The paper does not address differences in electricity tariffs, but rather assesses total electricity costs of the plant. The authors even find that energy prices have a minor impact on energy consumption compared to other process parameters in their model. However, the authors acknowledge the importance of investigating the effect of different electricity tariffs on energy consumption in the future.

Table 3: WWTP models investigating DR

	Publication	**Subject of analysis**	**Methodology**
Model based	Póvoa et al. (2017)	Cost efficiency of control strategies	ASM1
	Emami et al. (2018)	Effect of influent on energy costs	Biokinetic model and aeration submodel
	Aymerich et al. (2015)	Effect of different energy tariffs on energy cost	ASM1
	Giberti et al. (2019)	Effects of demand shedding in aeration process on plant performance	ASM1
Data-driven	Asadi et al. (2017)	Cost optimisation of aeration control	Neural Network
	Torregrossa et al. (2018)	Energy cost models	Neural Network

It can be seen that in all models, DR activity is triggered by an exogenous price signal from the power market. All of the models above optimise the WWTP operation subject to a fixed electricity price pattern, either as flat tariffs or flexible tariff rates. There is no interaction between the electricity system operation and the WWTP operation. That means that while these models are suitable for investigating the effect of different price patterns on WWTP operation, investigating the effects of large-scale DR from WWTPs on the electricity system is out of the model scope.

2.4. Comparison between existing DR modelling approaches

The review of different modelling approaches shows that DR can be considered from different modelling perspectives. A summary of the identified differences between energy system models, industrial process optimisation and simulation models (which includes WWTP models) is given in Table 4.

Table 4: Energy system models and industrial process models compared

	Energy system models	Industrial process optimisation	Industrial process simulation (including WWTP models)
Mathematical approach	(MI)LP	(MI)LP	System of non-linear differential equations
Subject of analysis	System operation (supply side)	End-user operation (demand side)	Physical reactions and processes
Integration	End-users as black boxes	Closed system (energy price simulation)	Closed system
Model elements	Objective function and system constraints	Simplified process equations	Process rates and physical mass balance equations
Aim of model	System cost minimisation or welfare maximisation	Production cost minimisation, profit maximisation	Evaluation of control strategies
Time frame	Discrete time steps	Discrete time steps	Continuous time

Energy system models are used to investigate how DR affects the overall system operation. Process optimisation models focus on the end-user operating schedule considering DR provision. Process simulation models, such as the WWTP models presented here, provide insights about the inner physical processes. While energy system models and process optimisation models focus on cost optimisation, process simulations often aim at evaluating the cost effectiveness of different control strategies under a given energy pricing regime.

So far, industrial process models only account for exogenous energy price patterns, and energy system models do not account for end user processes in sufficient detail. Moreover, the disadvantages of neglecting the interaction between system and process operation have become eminent from the literature review. An integrated approach, combining energy system optimisation with the level of operational detail in process simulation models, could yield the highest level of accuracy regarding the DR potential from a specific process, such as wastewater treatment.

Problems arise from the different mathematical approaches of optimisation and simulation models. While energy system models are mostly formulated as an LP or MILP, process simulation models often use non-linear approaches. Therefore, a joint representation of the electricity system and a process like wastewater treatment in an integrated energy system is challenging. So far, research in the realm of the energy-water nexus has not yet tackled this challenge. Instead, a review of the literature on the energy-water nexus shows that existing models focus on overall system efficiency or the water requirements of the energy sector. For example, Chen and Chen (2016) apply an ecological network analysis framework for investigating water and energy consumption within the urban energy-water nexus of Beijing, China. Tsolas et al. (2018) use a generic graph-theoretic network approach that accounts for the interactions between energy and water flows to identify redundant subsystems and redesign the nexus for optimal resource generation and utilization.

Gabriel et al. (2016) consider the integration of industrial heat, power and water via hybrid thermal-membrane desalination. DeNooyer et al. (2016) analyse the current and future water requirements for cooling in thermal power generation in Illinois, using a geographic information systems (GIS) model. Yang et al. (2014) proposed a MILP to determine optimal water consumption in shale gas production. Santhosh et al. (2014) develop an ED model to co-optimise the dispatch of power generation and potable water treatment. They specifically allow for co-production of water and energy in a single utility, representing for example hydroelectric or thermal desalination, which can serve either the power demand, or the demand for potable water. Baliban et al. (2012) develop a mixed-integer nonlinear energy-water model for an industrial process that converts biomass, coal, and natural gas to liquid transportation fuels. The model accounts for fresh water requirements of the process and comprises wastewater treatment units that process and recycle wastewater.

This brief review reveals that energy-water nexus models dealing with the energy requirements of the water sector are underrepresented. In particular, we did not find a model that investigates the flexibility and DR potential from wastewater treatment plants.

3. Wastewater treatment as a DR resource

This section explores wastewater treatment as one promising application for industrial DR. First, we outline the energy demand of wastewater treatment in contrast to other water services. We identify the main energy consuming processes within a WWTP and explore case studies on their potential for DR provision in the following subsections.

3.1. Energy demand of water and wastewater processes

Energy is required to lift groundwater, desalinate sea water and pump and treat both freshwater and wastewater. Most of the energy consumed in fresh water supply and treatment is due to pumping and disinfection. In a conventional water treatment plant with coagulation, flocculation, sedimentation and filtration, the total energy requirement varies between 0.25 and 1 kWh per m^3 of treated freshwater (Gude, 2015). In general, the treatment of ground water or surface fresh water is not highly energy-intensive. In contrast, desalination of sea water or brackish water, which is sometimes necessary in dry regions with close proximity to the sea, is very energy-intensive. The process consumes up to 20 kWh per m^3 of treated water (Gude, 2015).

Water pumping is also the major energy-consuming process in the water distribution system. The energy consumption depends on the topology of the region, the quality of the infrastructure (for example, if there is a high amount of leakage in the pipe system), as well as the distances over which water has to travel to the consumers. Water consumption itself also often consumes additional energy, mainly for heating or cooling the water to a desired temperature.

Apart from desalination, wastewater treatment is the most energy-intensive process in the water cycle. Gude (2015) states that it typically requires between 0.5 and 2 kWh of energy to treat 1 m^3 of wastewater. The energy requirements for wastewater recovery, such that water can be reused for human purposes, are in a similar range. In the United States, wastewater treatment accounts for around 3 percent of total electricity consumption (Gude, 2015).

Most electric energy is required for the aeration in the activated sludge process and the wastewater pumping. Figure 4 shows the share of the electricity consumption in the influent pumping and the aeration process from the total energy consumption of plants with a conventional activated sludge (CAS) system, as monitored in different case studies. It can be seen that the aeration in the activated sludge process consumes the highest share of electricity, ranging between 10.2 and 71 percent of total electricity consumption. Depending on the topology of the plant, the inflow pumps consume up to 15 percent.

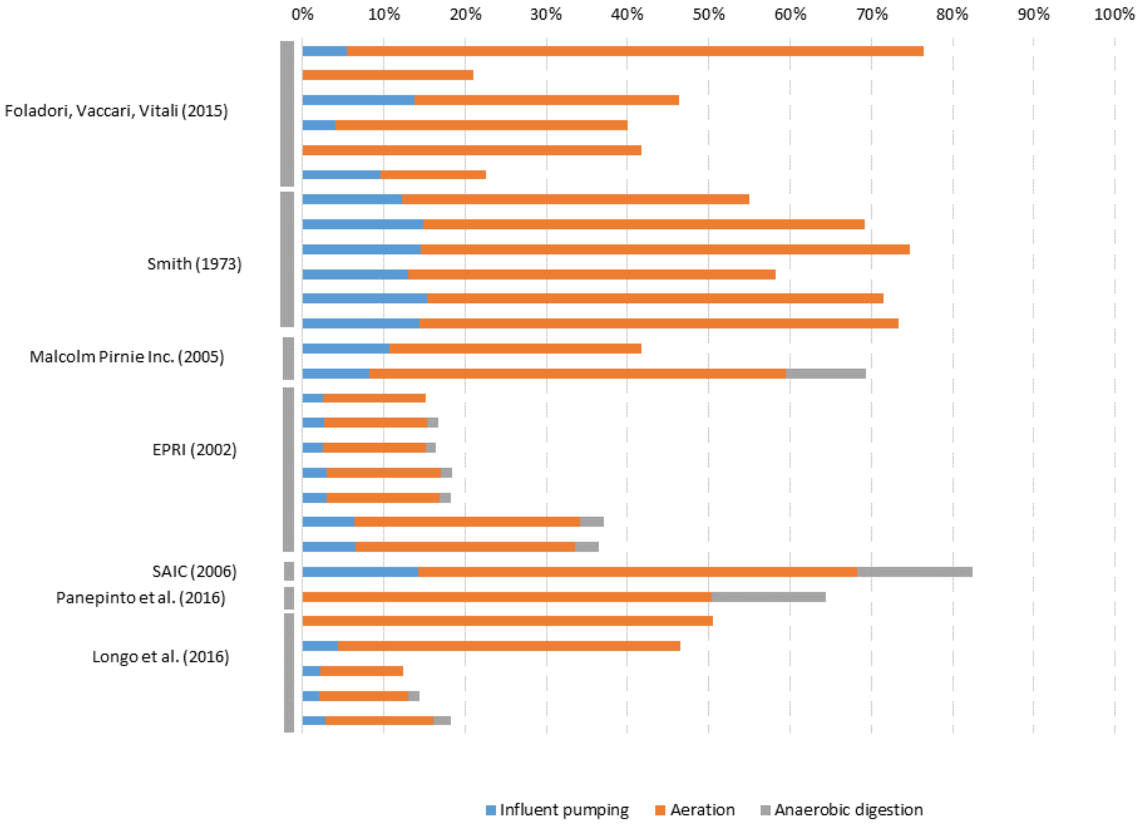

Figure 4: Share of total energy consumption across case studies (Foladori et al., 2015; Smith, 1973; Malcolm Pirnie, 2005; EPRI, 2002; SAIC, 2006; Panepinto et al., 2016; Longo et al., 2016)

Therefore, many studies have performed energy audits (see some examples in Table 5), looking into the possibilities to improve energy efficiency (Foladori et al., 2015; Guerrini et al., 2017) and to save energy in pumping and aeration (Awe et al., 2016; Panepinto et al., 2016). Fewer studies explore the technical potential for flexibility and assess the economic potential of changing the operating schedule according to energy prices.

Table 5: Energy audits of WWTPs

Data type	Energy audits	Country	Number of plants
Total energy consumption	Silva and Rosa (2015)	Portugal	17
(and biogas production)	Bodik and Kubaska (2013)	Slovakia	51
(and other cost factors)	Hernández-Sancho et al. (2011)	Spain	177
Total energy costs	Guerrini et al. (2017)	Italy	127
	Póvoa et al. (2017)	Portugal	1
Energy consumption of subprocesses	Foladori et al. (2015)	Italy	5
	Longo et al. (2016)	Multiple	601
	Awe et al. (2016)	Ireland	1
	Panepinto et al. (2016)	Italy	1
	Wett et al. (2007)	Austria	1
	Schäfer et al. (2017)	Germany	1

3.2. Energy demand flexibility of wastewater treatment

There is a slight tendency towards load shedding strategies across the reviewed case studies that explore the flexibility potential for WWTPs. However, the potential for load shifting is also addressed in some publications. The opportunities for flexible operation are investigated for the aeration in the activated sludge and for wastewater pumps at several stages of the treatment process in conjunction with the use of overcapacity in the tanks (Schäfer et al., 2017; Aghajanzadeh et al., 2015). Anaerobic sludge digestion, which is a part of many modern WWTPs, also allows for flexible operation. Additionally, the process generates biogas, mainly methane, which can be used to produce electricity on-site.

The flexibility options reviewed are the sludge processing, the aeration process, the wastewater pumping and the use of built-in redundancy. Since the aeration and the pumping consume significant amounts of electricity, they can be classified as flexibility options that can be used to provide DR. In contrast, one can argue that the flexibility provided by biogas production cannot be classified as a DR action, since the flexibility does not arise from load shedding or load shifting of an electricity-consuming process, but rather from the production and self-consumption of electricity. However, the ability to produce electricity on-site affects the energy consumption from the grid and consequently the DR provision. Therefore, the flexibility options within the sludge processing are reviewed first, followed by the flexibility potential of the aeration process and the pumping. We also explain how the use of built-in redundancy affects the flexibility potential of the pumps.

Sludge processing

Sewage sludge is a by-product of the wastewater treatment process. It refers to the solid part of the wastewater that settles down in the tanks and is generally disposed to landfill or used for land applications. Prior to disposal, the sludge needs to be dried in several steps in order to reduce its volume. This sludge treatment can account for about 30 percent of a plants operating costs (Shen et al., 2015). After thickening the sludge, it enters the anaerobic digestion system, normally consisting of a reactor filled with liquid sludge, and a sealed gas headspace (Batstone et al., 2002). The biochemical and physico-chemical reactions within the sludge release biogas to the headspace, which can be extracted into storage tanks for further utilisation. Afterwards, the remaining sludge is dewatered, typically in a centrifuge, for final disposal. Figure 5 depicts the sludge treatment process.

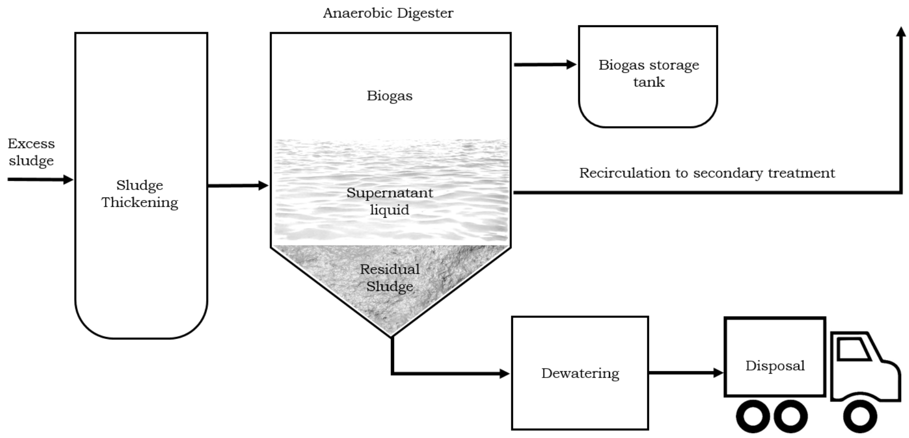

Figure 5: Sludge treatment process

The biogas captured in the tank's headspace can be transformed into electrical (and thermal) energy by a combined heat and power (CHP) plant or used as a transport fuel. The electric energy produced by an on-site CHP can either be used to drive the aeration system or heat the sludge digesters (Wett et al., 2007). Shen et al. (2015) claim that biogas recovery from sewage sludge has the potential to make a WWTP energy self-sufficient and even turn it into a net energy producer. However, significant capital and maintenance costs are connected with the implementation of an on-site electricity generation system, which can be a high barrier for WWTP operators to implement a CHP system.

Schäfer et al. (2017) finds the greatest flexibility potential within a WWTP in Germany in the operation of a CHP unit fed by biogas from the anaerobic digestion. Based on this, Schmitt et al. (2017) calculate a total flexibility potential for WWTPs in Germany of 2,057 MWh/day of additionally available load and 2,391 MWh/day of curtailable load for the whole treatment process. The majority of this flexibility is based on the availability of CHP for on-site electricity generation. Seier and Schebek (2017) find that German WWTPs, which use biogas for electricity generation, have a potential to integrate 120 MW of surplus electricity. Gude (2015) estimates that biogas produced from anaerobic digestion can cover up to 50 percent of the total energy needs for sludge treatment and that WWTPs can even become net energy producers if energy recovery rates from biogas increase.

The aeration process

The aeration process is an essential part of a CAS system, which is the most common treatment technology among WWTPs with secondary treatment. The injection of air into the reactor tanks supports the growth of microorganisms that break down the organic and nitrogenous matter in the wastewater (Aghajanzadeh et al., 2015). The two main methods of aerating wastewater are mechanical surface aeration, where the water is aerated by agitation of the water surface, and the use of submerged diffusers to inject air or pure oxygen directly into the wastewater (Bolles, 2006). In the activated sludge process, diffused aeration systems are most commonly used. They typically consist of blowers, air pipes and diffusers (Brandt et al., 2006). The size and number of blowers and diffusers is determined by the biological oxygen demand (BOD) of the wastewater and by the efficiency of the equipment (Aghajanzadeh et al., 2015).

In CAS systems, the aeration within the aerated tank is a continuous process in order to provide a stable environment for the bacteria which perform the organic decomposition. Other treatment technologies, e.g. the sequencing batch reactor (SBR), employ a strategy of intermittent aeration in order to create a cycle of anoxic and aerobic conditions within the tank (Tchobanoglus et al., 2003). This illustrates that the required energy for aeration highly depends on the type of treatment technology. Additionally, factors such as the population of aerobic bacteria, the pollutant loading of the wastewater, the standards for effluent quality, and the size and age of the treatment plant play an important role (Awe et al., 2016). Seasonal variations of inflow patterns and weather conditions also determine the aeration requirements. On the one hand, the overall wastewater inflow is lower during dry months (Lekov, 2009), which reduces the aeration requirement e.g. during summer. On the other hand, it has to be taken into account that the DO concentration is a function of temperature (Tchobanoglus et al., 2003). With higher temperatures, the oxygen demand for biochemical reactions increases (Aghajanzadeh et al., 2015), which means that maintaining DO levels requires more extensive aeration during summer months (Tchobanoglus et al., 2003). Determining the optimal operating schedule of the aeration process requires the consideration of all these factors.

Several case studies find that shutting down the aeration in peak periods is possible for a limited amount of time without a significant change in effluent quality. Schäfer et al. (2017) conduct a case study on a German WWTP and find that the aeration can be switched off for 60 minutes without a significant decline in effluent quality, with a maximum effective power flexibility of 98.6 kW. Müller and Möst (2018) find that the aeration can be turned down for 30 minutes at maximum at day-time and up to 120 minutes during night-time. Nowak et al. (2015) come to a similar result, turning off the aeration for a period of 60 to 120 minutes without breaching the effluent standards. In contrast, Berger et al. (2013) and Kollmann et al. (2013) evaluate a possible switch-off duration of only 15 minutes. In another case study of a California WWTP by Thompson et al. (2010), switching off the aeration for 120 minutes negatively affected the effluent turbidity. The study of Giberti et al. (2019) also emphasises the potential negative effects of load shedding on effluent turbidity. This shows that the technical flexibility of plant equipment can vary significantly.

Thompson and McKane (2008) propose the idea of excessive aeration during off-peak periods to extend the switching-off time during peak periods. This is based on the idea that the DO concentration within the water can be increased by over-aerating the water. Ideally, this could extend the phase in which the DO concentration is decreasing when the aeration is off, down to a critical level when the aeration has to be switched back on. To our knowledge, there have not yet been any case studies of WWTPs to test for its feasibility. Neither have there been any attempts to model over-aeration to investigate its DR potential. However, Brdjanovic et al. (1998) demonstrates the negative impact of excessive aeration on the process efficiency, namely the biological removal of phosphorus. The fact that only a limited amount oxygen can be dissolved in water (Tchobanoglus et al., 2003) might restrain the flexibility potential even further.

Wastewater pumping

Wastewater pumping is often the second most energy-intensive process in a WWTP after the aeration (Awe et al., 2016). Pumping is necessary in the form of inlet pumps, because topographic conditions often prevent the wastewater from flowing into the WWTP naturally. Even in the case of favourable topography, inlet pumps are often in place due to the texture of the sewage, that results in an innately slow flow rate. Additionally, sludge recycle pumps are used to recycle a part of the sludge from the secondary clarifier back into the aerated tank (see figure 1). This is necessary to maintain the bacteria concentration within the aerated tank. Both processes have been subject to research to explore their potential for load shedding and load shifting.

In the case study of Schäfer et al. (2017), it was possible to switch off the sludge recycle pumps for 120 minutes without a negative effect on the effluent quality, providing a maximum of 23.6 kW of effective power for flexibility. According to a case study in California from Olsen et al. (2012), lift pumps and external pump stations show potential for load shifting, because of their low ramp rates.

Many studies investigate how to operate pumps in WWTPs with minimum energy consumption (Torregrossa et al., 2017; Zhang et al., 2012; Chang et al., 2012; Olszewski, 2016). However, there is not yet much published research on the potential for load shedding or load shifting of inlet or recycle pumps. An important condition for pausing wastewater pumping in peak periods is that wastewater can be withheld in the system to a certain extent, either in tanks or in the pipes. Many WWTPs have built-in redundancy on-site, which can potentially be used in order to operate pumps intermittently.

Using built-in redundancy

Particularly small-scale WWTP often have redundancy on-site, in the form of oversized or additional tanks or overcapacity in the sewers. WWTPs can extend the retention time of untreated, partially treated or treated wastewater during peak periods and process or release it later during off-peak hours (Aghajanzadeh et al., 2015), if site conditions allows for longer wastewater retention. In the energy audit performed by Foladori et al. (2015) (see figure 1), the design capacity of all WWTPs exceeds the capacity which is actually used for treatment. Schäfer et al. (2017) find in their energy audit that small-scale WWTPs have more unused capacity than larger WWTPs, due to oversized equipment. Furthermore, large WWTPs are often already operated at optimised level, while small WWTPs often operate below design capacity. This is often due to a lack of adequate monitoring devices in smaller plants.

The study by Olsen et al. (2012) finds potential for flexibility in pumping due to overcapacity in the San Francisco sewer system and the WWTP. Findings suggest that lift pump could be curtailed for several days. However, the authors emphasise that the redundancy serves the purpose to account for the risk of heavy rain fall events. Using it for the provision of DR means that the safety margin given by redundancy decreases. An unanticipated exposure to a sudden rainfall event when sewers and tanks are already heavily loaded increases the risk of over-stressing the system and discharging untreated wastewater. Therefore, they conclude that the use of redundancy for DR must be evaluated carefully based on high-quality weather forecasts.

4. Discussion

Potential of DR from WWTPs

The potential of industrial DR has been considered in several studies. Cappers et al. (2010) state that 14,800 MW of the existing DR customer base in the US comes from the industrial sector, while the residential sector provides about 6,000 MW of DR resources. Gils (2014) estimates the theoretical DR potential for Europe, including 30 different electricity consuming sectors with a load shedding or shifting potential of a minimum of one hour. Findings suggest that processes with short intervention times, such as cooling, air conditioning and wastewater treatment, show the biggest potential for DR. Wang and Li (2015) conduct a survey of 43 ToU pricing schemes for industrial customers in the US. They point out that customers that do not adjust their production schedule when switching from a flat to a ToU tariff, can ultimately face higher electricity costs. Therefore, cost savings range from -72.0 to +82.6 percent, depending on the adaptability of the production schedule.

Wastewater treatment is an electricity-intensive industrial process and a coordinated DR programme for WWTPs could have a significant impact on the power system. The participation in DR programmes is potentially beneficial for the plant operators in order to achieve savings in electricity costs by making use of time-varying electricity rates. The implementation of the options presented in section 2 (excluding the installation of a CHP plant for on-site electricity generation) do not require significant investments in additional technology, which could hamper the net cost savings. Wastewater flows follow a diurnal pattern that coincides with electricity demand patterns, with one peak in the late morning and another one during the early evening between 7 and 9 pm (Thompson and McKane, 2008). If wastewater treatment is carried out according to this pattern, the electricity demand of the WWTP is high when overall system demand is high. Under a TOU tariff regime, a shift of treatment from peak to off-peak periods, for example from evening to night times, can yield electricity expenditure savings. The scope of potential savings depends on the degree of shiftable load. For example, Aghajanzadeh et al. (2015) estimate that the participation in DR programmes can provide energy cost savings of up to 15 percent by shifting loads from peak to off-peak periods.

Specific characteristics of industrial customers can limit the potential for DR. The energy infrastructure (electricity meters and sensors) on site, the intertemporal interdependency of production processes and the precision in timing that some processes require (Samad and Kiliccote, 2012) are the main limiting factors for the ability to react to a DR signal. The lack of adequate monitoring and control equipment is a challenge for small-scale WWTPs in particular. The expensive installation of meters and controls and ideally an automated control system can prevent plant operators from becoming DR providers. Concerns about revealing confidential and commercially-sensitive electricity demand data can also impede participation in DR programmes (Samad and Kiliccote, 2012). Furthermore, operating within environmental standards for effluent quality is a high priority within a WWTP. That means any deviation from the usual operating schedule can only be considered if the risk of discharging water of insufficient quality is not increased.

The quantification of the potential of DR from WWTP is essential to evaluate its value added for the power system and market. The case study by Schmitt et al. (2017) indicates that DR provision by WWTPs supports the integration of more RES into the power system. Harnessing the flexibility provided by the WWTP, the share of curtailed wind energy was reduced by 92 percent. The findings of Seier and Schebek (2017) suggest a total potential of German WWTPs to integrate 120 MW of surplus electricity. However, these findings are technology- and country-specific and cannot simply be applied to other energy systems.

A combined system-process model for DR from WWTP

The literature review shows that most DR system models do not specify the resource which is providing DR and focus on the system effects of DR. For this purpose, these models often take on the form of ED or UC. DR influences the energy demand in the system and ideally changes the daily load profile. This can improve the utilisation of renewable energy sources, which can be analysed by means of an ED or UC model. They can also be used for quantifying the economic cost and savings of DR. The underlying assumption of these DR models is that the system operator is capable of centrally co-optimising the dispatch of demand-side resources and generators (Papavasiliou and Oren, 2012). As a result, the outcome of an ED or UC model provides a good benchmark for the DR potential, when assuming no strategic behaviour and information asymmetries among system participants.

However, understanding the DR potential of a specific industrial process requires a detailed process model which takes into account minimal production disruptions and production costs. These models often consider energy price signals to be exogenous. Following this approach, end-users are assumed to be price takers that do not have any influence on the market through changing the energy demand profile. However, a coordinated DR signal across multiple big industrial consumers is likely to influence overall system demand, and hence prices. These effects of DR on the energy system cannot be studied within the framework of a DR process model like the ones presented here. An integrated energy system should ideally incorporate both the relevant details of a process model and the power system to capture the potential for DR from a system perspective.

This literature review has shown that there is not yet a model which combines these two important aspects to perform a meaningful analysis of the DR potential from industrial processes such as WWTPs. The reason that most DR system models abstract from the physical processes within end-use applications lies in the non-linearity that characterises many of them. Standard ED and UC models are linear or mixed integer linear programmes, which cannot handle non-linearity in constraints. The wastewater treatment process in particular is characterised by complex biological and chemical reactions with a non-linear nature. The standard WWTP models, like the ASM1 model, capture these reactions well. However, these models are used for process and design simulations and integrating them into a linear optimisation framework is challenging. The constraints which determine the biological and chemical reactions within the WWTP would have to be simplified and linearised to find a balance between accuracy and computational cost. This has not yet been attempted for any WWTP model. We have also shown that none of the multi-sector energy system models deals with DR potential within the energy-water nexus yet. Coupling energy sectors, and especially the electricity and water sector, within an energy system framework is not yet in the focus of DR research.

There is no study that investigates the DR potential from WWTPs in an integrated energy system so far. Although studies such as Seier and Schebek (2017) assess the DR potential from WWTPs, they do not take on a power system perspective, but rather perform a cost minimisation from the plant operator's perspective, with an exogenous electricity price signal. They also assume biogas storage and use for on-site electricity production as the only source of flexibility. In order to analyse all of the flexibility options summarised in this paper comparatively, an integrated energy-water system model of the wastewater treatment process and the power system is required. To our knowledge, such a model does not exist to date.

Our future contribution will be to develop a novel integrated energy systems model, which can account for the process detail of industrial end users traditionally only provided by process simulation models. Taking WWTP as an example for an industrial end user process, this will be achieved by coupling the traditional MILP approach for power systems modelling with a simplified and linearised WWTP model. Within this framework, the DR potential from WWTPs can be identified not only for the plant operator, but also for the power system. Moreover, in contrast to existing WWTP simulation models, this novel approach accounts for interaction between the power system and the wastewater

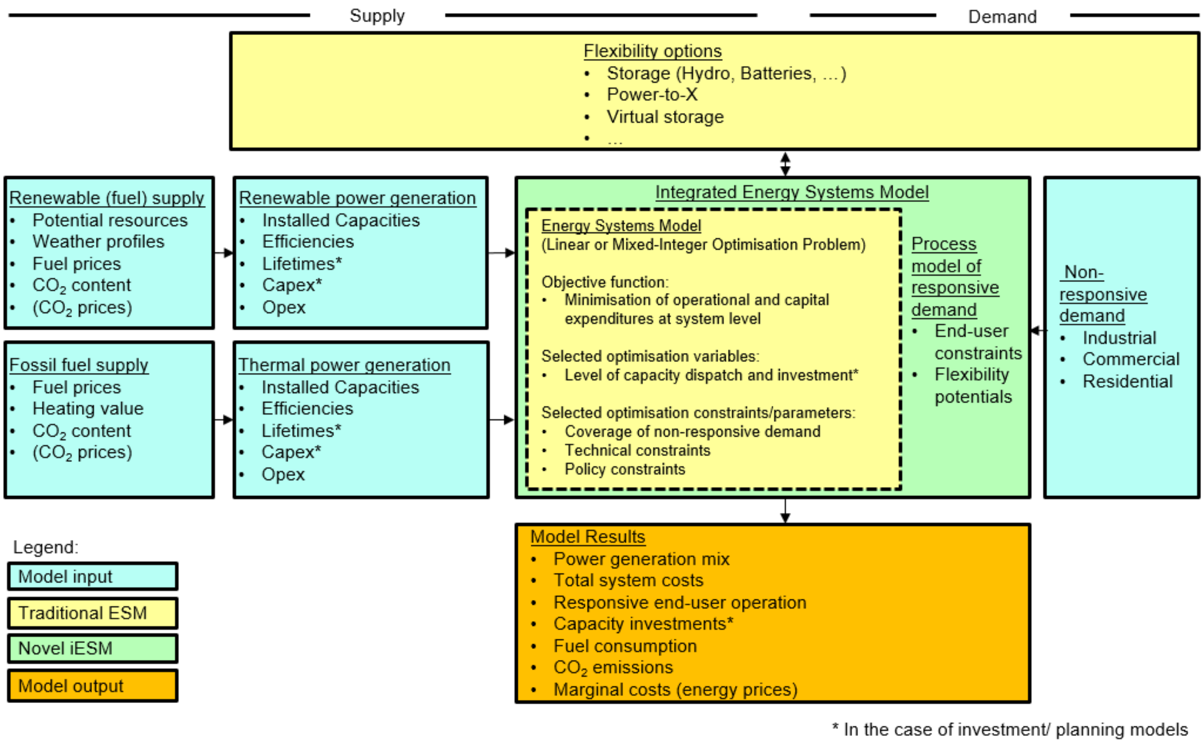

Figure 6: The novel integrated ESM approach

treatment sector caused by DR.

Figure 6 depicts the novel integrated energy systems approach required. Traditional energy systems models often employ a bilevel approach and determine the end user DR action with the help of a detailed process simulation model prior to the system level optimisation. In contrast, this approach includes detailed physical process constraints directly into the central optimisation problem. This ensures that the interaction between power system and end-user process are taken into account and thereby yields a more accurate estimation of the DR potential from the process.

Additionally, a detailed representation of the end-user process enables the assessment of the DR potential of different electricity consuming subprocesses within the industrial end user individually and combined. In the case of WWTPs, this would allow us to compare the DR potential from pumps, blowers and on-site redundancy and to identify the best DR strategy. Uncertainties regarding wastewater inflow rates, e.g. due to heavy rain falls, can be included into the analysis by using a stochastic approach. The described model will provide a framework for incorporating similar continuous end user processes into an energy system optimisation problem. Thereby, it is not only an important contribution to the existing literature on DR within the energy-water nexus, but also to the literature on DR modelling in general.

5. Conclusion

DR models can be grouped into two categories: energy (or power) system models, which take on a system perspective of the optimal utilisation of DR, and process scheduling models, which analyse the optimal DR strategies for a particular end-user. The reviewed energy system models often do not specify the DR resource in place, but rather assume a generic unit which provides DR. Meanwhile, industrial process models go into greater detail, but assume price signals from the power system to be exogenous. However, sufficiently large DR resources cannot be viewed as mere price takers. An increase in DR in a system can be interpreted as an increase in demand elasticity. With a more elastic energy demand, price changes can be induced by either the supply or the demand side. This endogeneity of prices is not yet captured in process models which deal with DR. Given the size of the wastewater treatment sector as one example of an industrial process with significant electricity demand, this endogeneity has to be taken into account in order to assess the DR potential accurately.

The two main reasons for over- or underestimating the available DR potential from an industrial end user have been identified by this review. The first reason is the neglect of the interaction between power system operation and industrial process operation caused by DR. The second reason is the abstraction from critical physical process constraints affecting the DR potential. None of the reviewed DR modelling approaches is currently capable of accounting for the interaction while providing enough operational detail of the respective end user process at the same time. Therefore, we propose an integrated modelling approach, combining energy system optimisation with the level of operational detail in process simulation models. This could yield a higher level of accuracy regarding the assessment of DR potential from a specific end-user process.

This integration of a given end-user process into an energy systems model depends on the particular characteristics of the process in question. The general principals underlying this model integration apply for all the end-user processes reviewed in this article. In order to provide one relevant example, we also included detailed discussion on how the end-user process of wastewater treatment might be integrated into an energy systems model. This particular example was motivated by several reasons: our findings that there is under-exploited DR potential from this particular end-user process, and the fact that the energy-water nexus as a source of DR has been neglected to date.

Several case studies explore the operational flexibility of different energy consuming processes within WWTPs, and find that there is potential for load shifting for several processes. However, there is a lack of assessment of DR potential and its environmental and economic effects on both WWTP operators and the power system due to an identified modelling gap. In order to address this, wastewater treatment process-related constraints based on these findings should be applied to an integrated energy systems model. Future research will deal with the development of such an integrated energy-water model which can account for the wastewater treatment operation and the operation of the power system simultaneously. The described model will provide a framework for modelling similar industrial processes within an integrated energy systems model. Therefore, this review is not only contributing to the existing literature on DR within the energy-water nexus, but also to the literature on industrial DR modelling in general.

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Appendix A. Representative equations of energy systems models

Here, we provide some simplified equations outlining economic dispatch (ED) and unit commitment (UC) models, which represent the majority of energy systems models. An example of a simple economic dispatch model may look as follow:

$$min(systemcosts_t) = \sum_i fuelcosts_{i,t} \tag{A.1}$$

$$s.t.$$

$$load_t - \sum_i gen_{i,t} = 0 \tag{A.2}$$

$$gen_{i,max} \geq gen_i \geq gen_{i,min} \tag{A.3}$$

The objective function in Eq. (A.1), which is subject to minimisation, is determined by the sum of fuel costs for power provision of each generator i. Eq. (A.2) determines the load balance constraint, while Eq. (A.3) sets the capacity limits for the power generation for each generator. The optimisation is then performed for each time step t. Additional constraints depend on the specification of the respective power system, for example regarding the provision of reserves or transmission constraints.

In a unit commitment model, the economic dispatch is solved intertemporarily. A simple mathematical formulation is given in the following.

$$min(systemcosts) = \sum_t \sum_i fuelcosts_{i,t} + startupcosts_{i,t} + shutdowncosts_{i,t} \tag{A.4}$$

$$s.t.$$

$$load_t - \sum_i gen_{i,t} = 0 \tag{A.5}$$

$$gen_{i,max} \geq gen_{i,t} \geq gen_{i,min} \tag{A.6}$$

$$startupcosts_{i,t} = startupcost_i \cdot (state_{i,t} - state_{i,t-1}) \tag{A.7}$$

$$shutdowncosts_{i,t} = shutdowncost_i \cdot (state_{i,t} - state_{i,t-1}) \tag{A.8}$$

Here, the objective function (see Eq. (A.4)) typically comprises the different intertemporal cost components of the power generation, such as fuel costs, start-up and shut-down costs for each generator i in each time step t. Other cost components like ramping costs can also be considered. The binary state variables in Eq. (A.7) and Eq. (A.8) determine whether a generator is switched on and thereby turn the problem into a mixed integer linear programme.

Appendix B. Representative equations of generic demand response

The most common methods of formulating demand response in a generic manner are load shifting or load shedding. There are several ways how this can be modelled, one option for each load shedding and load shifting will be presented in the following.

For load shedding, one generic option is to model a virtual power plant on the supply side with no fixed costs and an incremental cost equal to the cost of load shedding λ_{shed}. This means that part of the system load can be "met" by load shedding, with the trade-off arising from the saved generation cost of meeting an additional part of the demand via load shedding and the costs arising from providing load shedding. This changes the optimisation problem from (A.4-A.8) to:

$$min(systemcosts) = \sum_t \sum_i (fuelcosts_{i,t} + startupcosts_{i,t} + shutdowncosts_{i,t}) + loadshed_t \cdot \lambda_{shed} \tag{B.1}$$

$$s.t.$$

$$load_t - \sum_i (gen_{i,t}) - loadshed_t = 0 \tag{B.2}$$

, while Eq. A.6-A.8 remain unchanged. As can be seen, the load balance constraint becomes the total generation at time t and the amount of load shedding, both subtracted from the total demand at time t.

For load shifting, the flexible portion of the energy demand of the end user from the reference demand $DREF^t$ needs to be determined. This flexible part is represented by the maximum load that can be curtailed at once, dr^t_{down} (downward flexibility) and the maximum load that can be ramped up additionally dr^t_{up} (upward flexibility). Then, a generic formulation of the profit Π_{energy} from DR provision in a downward direction (following Devine et al. (2019)) for a DR aggregator can be:

$$\Pi_{energy} = \sum_t (dr^t_{down} - dr^t_{up} - DREF^t) \cdot \lambda^t, \tag{B.3}$$

with

$$\sum_{t=t'}^{t'+23} (dr^t_{down}) = \sum_{t=t'}^{t'+23} (dr^t_{up}), \forall t' \in \{1, 25, 49, ...\} \tag{B.4}$$

Analogous equations hold for DR provision in an upward direction.

The DR aggregator obtains revenue from load-shifting and faces the cost of meeting the consumer's reference demand $DREF^t$. The flexible portion of the demand can be shifted up or down, with the condition that the sum of the shifts must be equal to one over a given time horizon, 24 hours in this case. The total load-shifting performed by the DR resource is the net result of the sum of $dr^t_d own$ and $dr^t_u p$, the upwards and downwards change from the reference demand DREF at each time,t. The load balance constraint (A.5) is thereby adapted to:

$$\sum_{i,j} gen^{t,i,j} - DEM^t + DREF^t - dr^t_{up} + dr^t_{down} = 0 \tag{B.5}$$

, with DEM^t being the non-responsive part of the load.

Appendix C. Example of process model to be incorporated in an IESM: the ASM1 model

As an example for the case of wastewater treatment, the following differential equations can be found for example in Jeppson (1996). They describe the 10 processes which constitute the basic ASM1 model, excluding the process equations for the dynamics for alkalinity. These equations are often displayed in a matrix form, but this can be confusing to an unexperienced reader, which is why the equations are displayed in full in the following. The model involves 8 processes: the growth of biomass (3), the decay of biomass (2), ammonification of organic nitrate (1) and hydrolysis (2). The differential equations describe the dynamics of 10 state variables:

- heterotrophic biomass B_H
- autotrophic biomass B_A
- readily biodegradable substrate S_S

- slowly biodegradable substrate X_S
- inert particulates X_P
- particulate organic nitrogen X_{ND}
- soluble organic nitrogen S_{ND}
- ammonia S_{NH}
- nitrate S_{NO}
- oxygen S_O

Energy demand in a biological wastewater treatment system is dependent largely on the aeration which is provided to supply oxygen. As can be seen with the following model, the oxygen demand is dependent on a number of variables which relate to the wastewater composition, flow-rate and reaction kinetics.

The dynamics of the heterotrophic biomass concentration are affected by aerobic and anoxic growth, and decay. The process can be described by:

$$\frac{dX_{B,H}}{dt} = \left[\hat{\mu_H} \cdot \left(\frac{S_S}{K_S + S_S}\right) \left\{ \left(\frac{S_O}{K_{O,H} + S_O}\right) + \eta_g \left(\frac{K_{O,H}}{K_{O,H} + S_O}\right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right) \right\} - b_H\right] X_{B,H} \tag{C.1}$$

Since autotrophs do not grow in anoxic environments, the description of the autotrophic biomass concentration lacks the part for anoxic growth. Therefore, the process equation is:

$$\frac{dX_{B,A}}{dt} = \left[\hat{\mu_A} \left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right) \left(\frac{S_O}{K_{O,A} + S_O}\right) - b_A\right] X_{B,A} \tag{C.2}$$

The dynamics of the readily biodegradable substrate concentration are influenced by the growth of heterotrophic bacteria and by the hydrolysis of slowly biodegradable substrate. The respective process equation is

$$\frac{dS_S}{dt} = \Bigg[-\frac{\hat{\mu_H}}{Y_H}\left(\frac{S_S}{K_S+S_S}\right)\left\{\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_g\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right\}$$
$$+ k_h\cdot\frac{X_S/X_{B,H}}{K_X+(X_S/X_{B,H})}\left\{\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right\}\Bigg]X_{B,H} \quad \text{(C.3)}$$

The concentration of slowly biodegradable substrate is increased by the recycling of dead bacteria and decreased by hydrolysis:

$$\frac{dX_S}{dt} = (1-f_P)(b_H X_{B,H}+b_A X_{B,A}) - k_h\frac{X_S/X_{B,H}}{K_X+(X_S/X_{B,H})}\left\{\left(\frac{S_O}{K_{O,H}+S_O}\right)\right.$$
$$\left.+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right\}X_{B,H} \quad \text{(C.4)}$$

The concentration of inert particulates products is described by the decay of biomass:

$$\frac{dX_P}{dt} = f_P(b_H X_{B,H}+b_A X_{B,A}) \quad \text{(C.5)}$$

Particulate organic nitrogen is increased by the decay of biomass and decreased by hydrolysis:

$$\frac{dX_{ND}}{dt} = (i_{XB}-f_P i_{XP})(b_H X_{B,H}+b_A X_{B,A}) - k_h\frac{X_{ND}/X_{B,H}}{K_X+(X_S/X_{B,H})}$$
$$\left\{\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K+NO+S_{NO}}\right)\right\}X_{B,H} \quad \text{(C.6)}$$

The development of the soluble organic nitrogen concentration is characterised by ammonification and hydrolysis, such that

$$\frac{dS_{ND}}{dt} = \left[-k_a S_{ND} + k_h\frac{X_{ND}/X_{B,H}}{K_X+(X_S/X_{B,H}}\left\{\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right\}\right]X_{B,H} \quad \text{(C.7)}$$

The ammonia concentration is affected by growth of all microorganisms and decreased by nitrification. Further, the ammonification of soluble organic nitrogen increases the concentration. The respective differential equation is:

$$\frac{dS_{NH}}{dt} = \left[-i_{XB}\hat{\mu_H}\left(\frac{S_S}{K_S+S_S}\right)\left\{\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_g\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right\}+k_aS_{ND}\right]X_{B,H} - \hat{\mu_A}\left(i_{XB}+\frac{1}{Y_A}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A} \quad \text{(C.8)}$$

The concentration of nitrate is increased by nitrification and decreased by denitrification. Its dynamics are described as

$$\frac{dS_{NO}}{dt} = -\hat{\mu_H}\eta_g\left(\frac{1-Y_H}{2.86Y_H}\right)\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)X_{B,H} + \frac{\hat{\mu_A}}{Y_A}\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A} \quad \text{(C.9)}$$

Finally, the oxygen concentration is reduced by the aerobic growth of heterotrophic and autotrophic biomass:

$$\frac{dS_O}{dt} = -\hat{\mu_H}\left(\frac{1-Y_H}{Y_H}\right)\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)X_{B,H} - \hat{\mu_A}\left(\frac{4.57-Y_A}{Y_A}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A} \quad \text{(C.10)}$$

The accurate modelling of the DR potential from an end user process such as WWTPs involves replacing or constraining the generic representation of DR in appendix B with the end-user process model, such as the ASM1 model shown here.

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