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Modelling Closed-Water Loops in the Process Industries

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Abstract Global water scarcity poses a significant challenge for the process industry, especially in water-stressed areas. Population growth and rapid industrialization make evident the necessity to incorporate sustainable and efficient water management strategies in the industrial sector. This study aims to point out the complex industrial systems at different levels presenting the modelling of them. Overall, three modelling levels are identified, i.e., in-process, in-factory, and systemic modelling based on the system's characteristics, requirements, and prospects. Individual process units, a series of water and wastewater treatment processes, a whole industrial plant and synergistic collaborations are modelled. In this regard, a generic methodology was developed in order to be applied in six discrete use cases, recommending the most appropriate model to be applied.

Keywords: wastewater treatment, process industry, modelling, sustainability

1. Introduction

The total available water reserves are approximately 1386 million km^3, but freshwater corresponds only to 2.5 % of this amount (Meran et al., 2021). Freshwater resources are becoming increasingly scarce and vulnerable to depletion, largely due to population growth, climate change, and increasing industrial water demand. Water is essential to the industry since the majority of the industrial treatment processes require a vast amount of water (Muralikrishna & Manickam, 2017).

Industrial production processes result in the generation of significant amounts of wastewater (Davis & Rosenblum, 2021). The discharge of effluents into the environment is an emerging environmental issue (Ranade & Bhandari, 2014). Surface waters, rivers, streams, and lakes are common water bodies where industrial wastewater is being disposed of (Davis & Rosenblum, 2021).

These industrial effluents have the potential to be treated, aspiring to reuse and recycle practices. In addition, the recovery of resources is of crucial importance. This approach could result in fewer raw materials, including water and other resources, and waste (Guerra-Rodríguez et al., 2020). The exploitation of alternative water sources can also lead to decreased freshwater intake and a more sustainable industrial sector (Date et al., 2022). Hence, a circular economy (CE) approach should be implemented in the process industry and especially in wastewater treatment (Guerra-Rodríguez et al., 2020).

To this end, industrial reuse and recycling practices are required (Davis & Rosenblum, 2021). The reuse of resources is achieved through wastewater treatment (Capodaglio, 2020). However, the reclaimed water must meet specified quality requirements before reuse (Davis & Rosenblum, 2021). For this reason, control systems and models are needed in wastewater treatment systems, aspiring to predict and enhance their performance (Capodaglio, 2020; Seco et al., 2020).

Furthermore, the creation of synergistic collaborations among process industries, which operate in the same or different fields, and other companies, e.g., the municipality, focuses on exchanging water and other raw materials. By-products are utilized within the developed network of interrelated actors, converting the effluents of one actor into the feed streams of another actor (Ashton et al., 2022). This way, they become more environmentally friendlier and sustainable, receiving economic benefits. This type of materials exchange is called industrial symbiosis and contributes to closing the loops by utilizing any produced waste (Henriques et al., 2022).

2. Materials and methods

2.1. Literature review

Several conventional and advanced wastewater treatment technologies have been studies over the last decades, including aerobic granular sludge (AGS) (Hou et al., 2021), adsorption (Sizirici & Yildiz, 2020), membrane bioreactor (MBR) (Al-Asheh et al., 2021), advanced oxidation processes (AOPs) (Pandis et al., 2022), ion exchange (IEX) (Hashemi et al., 2020), reverse osmosis (RO) (Tałałaj, 2022), pulse flow reverse osmosis (PFRO) (Liberman et al., 2020), ultrafiltration (UF) (Field & Wu, 2022), and coagulation/flocculation (CF) (Ehteshami et al., 2015).

The performance of these processes and the affecting factors have to be studied in order to develop mathematical models that can predict the removal efficiency in relation to specific contaminants from wastewater. Researchers have modelled the granular activated carbon filtration (Mozaffari Majd et al., 2022), aerobic granular sludge (van

Dijk et al., 2020), UV/H_2O_2 process (Hu et al., 2019; Rubio-Clemente et al., 2017), disinfection (Elhalwagy et al., 2021), membrane bioreactor (Deowan et al., 2019), reverse osmosis (Gaublomme et al., 2020), and ultrafiltration (Yang et al., 2021). Moreover, expanding the boundaries of the systems, the whole plant and the symbiotic relationships have been modeled. Aspects of CE (Mbavarira & Grimm, 2021), industrial symbiosis (Aviso et al., 2022; Huang et al., 2020) as well as the barriers to its implementation (Neves et al., 2019) have been studied. However, there is no research to our knowledge, which combines the different modelling levels in the process industry. Hence, the aim of this study is to present the identified levels and implement them into six case studies based on the developed methodological approach.

2.2 Methodology

Based on the literature review, the methodology presented in Figure 1 was developed to identify the most appropriate modelling level and the required steps for each use case. In this regard, the evaluation of the potential outcomes is feasible, facilitating the decision-making process.

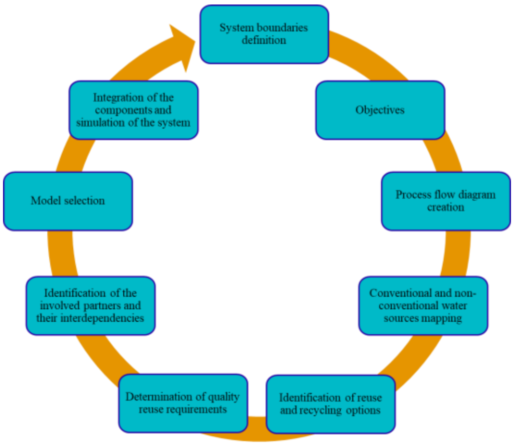

Figure 1. Methodological approach for modelling complex industrial systems

The methodology is implemented in the chemical industry of Dow in Terneuzen and Böhlen, Rosignano Solvay plant, and BASF. Also, the systems of the Agricola slaughterhouse plant and Tüpraş petroleum refinery are modeled.

2.3 Case studies description

Dow chemical company, Netherlands and Germany

Dow operates in the sector of chemicals and is located in a coastal area with limited availability of freshwater. For this reason, alternative water sources are examined, i.e., lake and river water as well as treated industrial effluents.

Rosignano Solvay plant, Italy

The Rosignano Solvay plant produces a variety of products, including plastic materials and hydrogen peroxide. It has created synergistic relationships with the municipal wastewater treatment plant and the Consorzio Aretusa through water and wastewater exchange. Thus, the optimal allocation of resources is a pivotal matter.

BASF chemical plant, Antwerpen, Belgium

The production plant of the BASF requires the abstraction of water from the docks of the area. Brackish water is used to fulfill the water demand. Industrial effluents and demineralized water are used within the plant. However, the high salinity levels make imperative their further water treatment before reuse.

Agricola slaughterhouse plant, Romania

Agricola International SA is a private meat group company, which produces approximately 150 tons of meat every day. Taking into consideration that the production of 1 kg of meat requires the consumption of 6 L of freshwater, the need for reuse and recycling practices through wastewater treatment with innovative technologies arises.

Tüpraş oil refinery, Turkey

Tüpraş produces 30 million tons of crude oil every year. However, it consumes vast amounts of freshwater. Thus, wastewater reuse after proper treatment is possible, considering that the reclaimed water meets the legislated quality reuse requirements.

3. Results and discussion

The different levels of modelling (Figure 2) emanate from the case studies and their requirements.

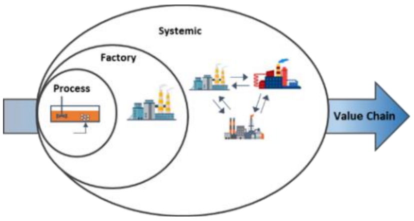

Figure 2. Schematic representation of the different modelling levels

The first modelling level refers to individual process units used for wastewater treatment. Water and resources recovery, reduced wastewater production and decreased freshwater intake are important aspects. To this end, mathematical models are developed to predict the performance of each treatment technology. The removal efficiency of industrial contaminants, effluent quality, chemical consumption and energy requirements are estimated by taking into account the process-specific parameters. Table 1 summarizes the technologies that have been modeled for all case studies.

The modelling of the treatment technologies predicts their removal efficiency and overall performance and is called in-process modelling.

If multiple units have to be modeled, for example in a wastewater treatment plant (WWTP), in-factory modelling is applied, which is the next level. The purpose is to detect the possible sources of water loss, e.g., due to evaporation, leakage or sludge production, decrease freshwater consumption, balance the water resources and improve the network's efficiency. Hence, water balances across the condensate grid of Dow, Netherlands, are formulated based on flow rates, Q (L/h), and the relevant concentration, C (mg/L). The generic equation for this modelling level is the following:

$$\frac{\mathrm{dC}}{\mathrm{dt}} \cdot \mathrm{V} = \mathrm{Q_{in}} \cdot \mathrm{C_{in}} - \mathrm{Q_{out}} \cdot \mathrm{C_{out}} - \mathrm{Q_{loss}} \cdot \mathrm{C_{loss}} + \mathrm{r_i} \cdot \mathrm{V}$$

where dC/dt is the concentration changes over time (mol/L/h), V the reactor volume (L), and r the reaction rate (mol/L/h). The subscript in refers to the input, out the output, loss the water loss, and i a specific contaminant.

Table 1. Overview of the modeled wastewater treatment technologies per case study

Case study	Wastewater treatment technology
Dow, Netherlands	(Biological)GAC
	UF
	RO
	Electrodialysis
	IEX
Dow, Germany	(Biological)GAC
	RO
	Electrodialysis
	CF
	IEX
Rosignano Solvay, Italy	Neutralization
	AOPs (Heterogeneous Fenton process)
	MBR
	GAC
	IEX
	Disinfection
BASF, Belgium	RO
	PFRO
	GAC
	IEX
Agricola, Romania	MBR
	IEX
	UV/H_2O_2
Tüpraş, Turkey	AGS
	UF
	Regenerated RO membranes

In case multiple actors participate in the system, i.e., in industrial synergistic collaboration, systemic level modelling is the proper model-based tool, which entails quality, quantity, tariffs, and reuse standards of water. At this level, the partners exchange freshwater, wastewater and/or other resources instead of discharging them into the environment. Thus, the environmental impact decreases. The interested partners could be process industries, private and public companies of the same or different sectors. The goal is to find the most beneficial solution by evaluating alternative scenarios. The Rosignano Solvay plant exchanges its wastewater with the municipality and the wastewater reclamation plant (WWRP) of Aretusa. After the advanced industrial wastewater treatment with the pilot-scale WWTP of Solvay, there are three alternative closed-loop scenarios, as described in Figure 3, in order to reuse water with specific quality criteria. The pilot-scale WWTP of Solvay consists of the technologies described in Table 1. The alternatives options are:

- The first option is to send the treated wastewater to the municipality for secondary treatment and then to Aretusa for tertiary treatment. The produced water will be reused in the Solvay plant for cooling purposes.
- The second option entails the exchange of wastewater between Solvay and WWRP Aretusa. After the tertiary treatment, the reclaimed water is exploited within the industrial boundaries.
- The third option is to mix the effluent of Solvay with water provided by Aretusa in a variable ratio based on wastewater composition. Thus, the mixed stream substitutes partially for freshwater.

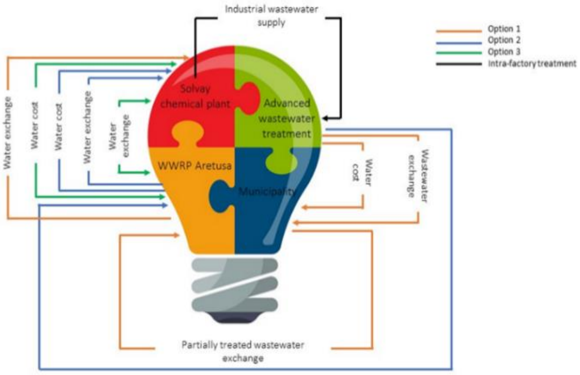

Figure 3. Systemic level modelling and the interdependencies among the involved actors

The systemic modelling will indicate the optimal scenario, considering the water reuse requirements for cooling purposes, e.g., for the cooling towers, and the economic factors since materials exchange is interrelated with a cost.

4. Conclusions

Water management is a challenge for the process industry. The concept of CE requires the adoption of different modelling levels (in-process, in-factory, systemic) based on case-specific requirements. Freshwater intake reduction, lower environmental impact, less wastewater production through synergies, reuse and recycling practices are crucial aspects in the industrial sector. Hence, fit-for-purpose closed-loop approaches have to be implemented, reinforcing sustainability.

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