



Municipal wastewater reclamation: Reclaimed water for hydrogen production by electrolysis – A case study

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ARTICLE INFO

Keywords:

Green hydrogen
Electrolysis
Wastewater treatment
Municipal wastewater

ABSTRACT

This paper presents an analysis of a treatment system selection for municipal wastewater stream based on the DuPont Water Solutions WAVE software. The results obtained based on an analysis of 7 different processing cases studies (ultrafiltration and reverse osmosis) confirmed that the application of 2-pass membrane systems enables the reclamation of water from municipal wastewater that fulfills the requirements concerning the quality of water intended as electrolyzer feedstock, as the obtained water exhibited a conductivity of $< 5 \mu\text{S}/\text{cm}$. Depending on the analyzed case study, the attainable level of water reclamation ranged from 68.8 to 84.1 % at an energy consumption of 606.1 – 2 694 kWh/d. The results of this work not only confirm that the selected processing solutions make it possible to reclaim water from municipal wastewater, but also confirm the necessity of using software to simulate the membrane system operation to select the most economic and cost-effective solution.

1. Introduction

With the increasing global population, water resource management should be approached unconventionally, and unused water resources should be diversified to limit the problems of deteriorating water quality and decreasing potable water reserves [1,2]. Unused water resources include e.g. wastewater, which may constitute an interesting source of drinking water as well as the water of a quality sufficient for processing purposes (process water) [3–7]. To prevent water scarcity in the European Union, the European Parliament has adopted Regulation (EU) 2020/741 of 25 May 2020 on minimum requirements for water reuse [8]. The purpose of this Regulation is to facilitate the uptake of water reuse whenever it is appropriate and cost-efficient, thereby creating an enabling framework for those member states who wish or need to practice water reuse. As per the Regulation, it is considered that the reuse of properly treated wastewater, for example from municipal wastewater treatment plants (WWTP), has a lower environmental impact than other alternative water supply methods, such as water transfers or desalination. Therefore, the necessity to identify alternative methods for water reuse or secondary wastewater treatment is justified.

The currently applied conventional methods of municipal wastewater treatment are not designed for wastewater reuse [9,10]. Conventional municipal wastewater treatment technologies include

mechanical biological methods, such as slurry removal on sieves and in settling tanks (mechanical methods) as well as through activated sludge microorganisms or biofilms (biological methods) [10,11]. In recent years, problems with access to clean and safe water as well as the global water crisis and strict legal regulations in waste management have forced municipal facilities to reconsider and implement third- and fourth-degree wastewater treatment. Examples of interest in secondary wastewater treatment processes include municipal facilities worldwide, e.g. the Waldwick wastewater treatment plant (New Jersey, USA) [12] or the Point Loma wastewater treatment plant (San Diego, USA) [13]. The Waldwick WWTP conducts secondary wastewater treatment using processes involving ultraviolet lamps to achieve the ultimate wastewater disinfection without the necessity of applying chlorine. By 2025, the Point Loma WWTP plans to produce about 129 000 m³/d of potable water from municipal waste by utilizing biological processes (biological activated carbon), membrane processes (microfiltration, reverse osmosis) and advanced oxidation (UV radiation, ozone, hydrogen peroxide). The application of secondary treatment processes depends on a WWTP's location (e.g. recreational areas, housing infrastructure, industrial areas, protected land, agricultural areas), therefore the end goals of secondary treatment may include e.g. agricultural irrigation, street and square cleaning, process water production for equipment cleaning, aquifer recharging by injection wells. The research work and

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new method investigation in this field led for example to the introduction of an installation for secondary wastewater treatment and pharmaceutical substance elimination at the Neugut WWTP in Switzerland [14,15]. The Neugut plant was the first wastewater treatment plant in Switzerland to implement full-scale ozonation. The conventional wastewater treatment system (primary settling tank, biological treatment, sand filtration) was expanded by an additional ozonation stage, which yielded a contaminant removal rate of about 80 %.

To fully close the water and wastewater circulation in a WWTP and to ensure its independence from the power supply, seeing as the price of electricity has increased drastically during the energy crisis [16], it is crucial to undertake action to enable the recovery of organic substances from wastewater and sewage sludge for energy purposes [17]. Hydrogen can be produced by a variety of processes and energy sources. The types of hydrogen depend on its production process and can be categorised as follows [18]:

- **Grey:** Grey hydrogen is mainly produced by steam reforming of natural gas or coal gasification. The use of grey hydrogen implies significant CO₂ emissions, which makes these hydrogen technologies not part of a net zero CO₂ emissions policy [19].
- **Blue:** Blue hydrogen is produced by combining natural gas steam reforming technology with Carbon Capture Storage (CCS) or Carbon Capture and Utilization (CCU) technology. In this variant, the resulting CO₂ emissions are captured using CCS or CCU technology, making the hydrogen produced nearly emission-free (emissions are reduced by up to 95 %). In contrast to green hydrogen, blue hydrogen is not a completely emission-free product, as harmful methane enters the atmosphere during the extraction and transportation of natural gas [20].
- **Green:** Green hydrogen is produced using renewable energy. Green hydrogen is part of the sustainable energy transition concept. This form of hydrogen production is the most preferable in terms of zero-emission energy and transportation [21,22].
- **Turquoise:** Turquoise hydrogen is produced by the pyrolysis of methane. The main substrate for production is natural gas. However, the process is driven not by burning fossil fuels, but by electricity (the vast majority should come from renewable energy sources to make the process CO₂-neutral). With biomethane as the feedstock, the process could be zero-emission [23].

The literature also highlights brown (or black) hydrogen. Brown (black) hydrogen is hydrogen produced by coal gasification, where during combustion, carbon dioxide is emitted into the atmosphere. Coal gasification involves heating coal to temperatures reaching over 1273 K, resulting in the release of coke gas [24].

On the other hand, the reclaimed water may be used to produce hydrogen by electrolysis, as well as for practical purposes, such as supplying technical processes, cleaning streets and equipment, watering plants, or even as a source of potable water. When considering the perspectives for technological development in the context of hydrogen production, promising directions (in the coming few years) can include anaerobic fermentation, biomass gasification, electrolysis (with renewable energy sources), and photobiological methods [25–28]. Some of these processes are already used in the context of hydrogen (electrolysis), while others still require an adjustment of the current technical solutions (anaerobic fermentation). In the public utility sector, potential can be found in biomass gasification, hydrogen recovery from biogas generated by anaerobic sewage sludge processing, and electrolysis [29–38]. Water electrolysis is the most promising direction, and in the future, it will constitute the most widely supported method of hydrogen production in the European Union. The electrolysis process consists in separating hydrogen from water using electricity through electrolyzers. The most widely recognized technical option for hydrogen production is water electrolysis powered by electricity originating from renewable sources. Hydrogen produced through systems powered by electricity

obtained from renewable sources is defined as green hydrogen [39]. The costs of green hydrogen production can be lowered by the low costs of solar and wind power as well as technical enhancements [40,41]. For these reasons, green hydrogen from water electrolysis is gaining increasingly more interest. Furthermore, it is estimated that by 2030 it will be possible to reduce green hydrogen production costs by about 60 % [18]. Currently, about 96 % of global hydrogen production originates from processes involving fossil fuels (primarily steam methane reforming and coal gasification) [42–44]. Hydrogen production using electricity (including electrolysis) constitutes about 4 % of the total production. The most popular devices for hydrogen production by electrolysis are alkaline electrolyzers. Polymer electrolyte membrane (PEM) electrolyzers are also available on the market – compared to alkaline electrolyzers, they have lower power (200–1150 kW) and similar efficiency (65 % to 78 %). Meanwhile, solid oxide electrolyzers utilizing steam at a temperature within 973 to 1173 K are currently under development, which would be characterized by high efficiency (at a level of 85 %) [45,46]. The PEM electrolyzer technology constitutes an alternative to the more conventional alkaline electrolyzers. This technology exhibits several advantages compared to the older solutions, namely increased electrolyzer efficiency (56–73 %), the possibility of obtaining ultra-pure hydrogen (purity class >=5.0, i.e. >=99.999 %), and a more compact design [47].

In theory, 8.92 L of deionized water are required to produce 1 kg of hydrogen and 8 kg of oxygen [48]. However, considering the potential water losses and the use of water for cleaning the equipment, the actual water required to produce 1 kg of hydrogen by electrolysis is estimated at 13.5–15.0 kg H₂O, and may even reach up to about 22.4 kg/kg H₂ [49]. The cost of hydrogen production depends on the applied process scale, equipment and substrates. The greater the efficiency of the equipment, the lower the investment and operating costs [36]. For example, over a short period of electrolyzer operation, the production cost may amount to about US\$10.5/kg H₂. At longer periods of equipment operation, the production costs decrease to about US\$2.05/kg H₂ [38,50]. Generally, hydrogen production by electrolysis is competitive relative to other methods, e.g. sewage sludge pyrolysis or steam methane reforming [31]. For comparison, the estimated cost of hydrogen production by sewage sludge pyrolysis may amount to about US\$1.2–2.2/kg H₂ [51]. The cost of hydrogen production by steam methane reforming ranges from about US\$1.14/kg H₂ in the case of large systems to about US\$3.19/kg H₂ for smaller systems [31,52].

Regardless of the feedstock, the water supplying an electrolyzer must first be purified and demineralized. Current research [49] indicates that water from the public water network is the most appropriate source of water for electrolysis due to the lower supply risk, lower costs, and the lack of complex processes for obtaining legal permissions. However, given the global water crisis and the dynamically changing formal and legal conditions related to the necessity for obtaining the relevant hydrological legal permits to draw water from the public water network, and considering Regulation 2020/741 of the European Parliament [8], alternative opportunities and sources of water for electrolysis should be investigated. Therefore the economic, environmental, and social factors should be considered before any final decisions are taken. Literature data indicate that treated municipal wastewater may constitute an alternative source of water for supplying electrolysis [49,53]. An advantage of the water reclaimed from municipal waste is its low hardness compared to the water drawn from the public water network (potable water quality).

The water supplying an electrolyzer should meet the requirements for deionized water and exhibit a conductivity of < 5 μS/cm; therefore depending on the quality of the treated wastewater, the following treatment processes may be necessary: accelerated filtration, chemical treatment (pre-treatment before membrane processes), ultrafiltration (UF), nanofiltration (NF), reverse osmosis (RO), ion exchange (IE), electrodeionization (EDI). Treatment by reverse osmosis and ion exchange is commonly applied before electrolysis to produce water with a

sufficiently low conductivity.

The decision to select a technology for water production from municipal wastewater must be preceded by the appropriate physico-chemical and biological analyses of the wastewater and by determining the available volume of waste as well as the water demand, and not exclusively for water production by hydrolysis. Commercial software for selecting membrane modules, provided by their producers, such as e.g. Winflows (Suez), IMSDesign (Hydranautics), or WAVE (DuPont Water Solutions), is very useful in the process of designing the appropriate membrane system for water reclamation from municipal waste for the production of water intended as an electrolyzer feedstock. This work presents the process of separation system selection for water reclamation from municipal wastewater, comprising pre-filtration, ultrafiltration, and reverse osmosis, utilizing the WAVE software by DuPont Water Solutions. This work aims to select a municipal wastewater pre-treatment technology for producing water of the quality required in the process of electrolysis using the WAVE software. Various membrane process systems (ultrafiltration, reverse osmosis) for producing water of a purity class of at least 3, i.e. with a conductivity of under 5 $\mu\text{S}/\text{cm}$, were evaluated. The WAVE software has thus far not been applied for membrane process modeling in terms of producing water from municipal waste that would fulfill the requirements for electrolysis. The primary advantage of the selected software is the user-friendly interface and the possibility of robust user panel management. Furthermore, membranes available on the market can be modeled in the WAVE software, which is unique compared to other programs.

The purpose of this paper is to present the practical aspects of applying membrane process modeling software. The demand for the results of this work arises e.g. from the Communication from the Commission to the European Parliament, the Council, the European Economic and Social Committee, and the Committee of the Regions, "A Hydrogen Strategy for a Climate-Neutral Europe" [39]. For the hydrogen economy to be implemented effectively, it is necessary to enhance the capacity for conducting and advancing research, and consequently to introduce the developed solutions and technologies for utilizing hydrogen in power generation, transport, and industry, including the conduction of research on methods for obtaining and processing water for electrolysis. The tests performed as part of this work will allow water supply and sewerage companies to implement similar technologies in municipal and industrial sites within the scope of processes enabling secondary wastewater treatment for processing purposes (water reclaimed from waste as a source for producing hydrogen by electrolysis).

2. Materials and methods

2.1. Wastewater samples

The treated wastewater was sampled in 2022 from a wastewater treatment plant located in one of the cities comprising the Silesian agglomeration (Silesian Voivodeship, Poland). The wastewater treatment plant is continuously modernized to fulfill the requirements of local law and European Union Directives for WWTP with an efficiency of > 100,000 population equivalent (PE). The last major modernization took place in 2012 and resulted in an increase in nutrient reduction by optimizing the biological wastewater treatment process. The WWTP operates in a mechanical biological system. The mechanical part comprises bar screens, sand traps, and primary settling tanks, while the biological part consists of biological reactors. The tests were carried out in 2022 at the certified laboratories of the Central Mining Institute. To inhibit any biological activity in the sample and eliminate the adsorption of compounds on the glass vessel walls, the samples were stored at a temperature of 277,15 K until the time of analysis (for no longer than 48 h), in compliance with the standard [54]. The analyses were based on composite samples (three samples mixed together, from which the average value has been obtained), as per [55]. The physicochemical

parameters of the treated municipal wastewater are presented in Table 1.

2.2. Water requirements for electrolysis

The requirements concerning water (wastewater) quality vary depending on the electrolyzer manufacturer, but typically the production of very pure hydrogen requires deionized water [49], i.e. water free of all solutes and pollutants, as pollutants may influence the reaction by deposition in the electrolyzers, on the electrode surfaces and/or in the membrane. The electrolyzer feedstock conductivity recommended by the American Society for Testing and Materials (ASTM) should amount up to about 5 $\mu\text{S}/\text{cm}$, or equal to the parameters for type I or II water per the requirements of standard D1193-06 [56], which corresponds to a conductivity of up to about 0.056 $\mu\text{S}/\text{cm}$ and 1 $\mu\text{S}/\text{cm}$ respectively. It was assumed that an optimal processing system should enable the production of water with a conductivity no > 5 $\mu\text{S}/\text{cm}$, therefore according to ASTM's specification.

2.3. Modeling in the WAVE software

2.3.1. Design parameters of the tested wastewater

The treated wastewater parameters adopted for the modeling in WAVE are presented in Table 2. The treated wastewater was characterized by increased turbidity (>10 NTU), total suspended solids (TDS), manganese, and iron. The pollutant content in the wastewater exceeded the recommended maximum pre-RO pollutant index values. The final permissible pollutant index values depend on the manufacturer's instructions and the applied membrane types. Wastewater treated by mechanical biological processes constituted the source for producing deionized water with a conductivity no > 5 $\mu\text{S}/\text{cm}$. The wastewater treated before the membrane filtration process was characterized by turbidity lower than 20 NTU, total suspended solids under 30 mg/dm^3 , and a total organic carbon content under 20 mg/dm^3 . The adopted design temperature was 19 °C. The treated wastewater was pre-treated by pre-filtration processes on a sieve with a mesh of 100 μm and by ultrafiltration to an SDI of < 2.5. The application of an antiscalant was adopted to limit scaling – sodium hexametaphosphate ($\text{Na}_6\text{P}_6\text{O}_{18}$). The efficiency of a single production process was adopted at a level of 100 m^3/h of water reclaimed from wastewater. For the analyzed processing systems, at an average water recovery of 76.3 %, the municipal wastewater flow was about 133–145 m^3/h , depending on the processing system (with or without concentrate recycling).

2.3.2. Selection of wastewater treatment processes for reclaimed water

The technology selection was based on the instructions of membrane manufacturers, including Lenntech [57,58]. The average conductivity of

Table 1
Characteristics of tested wastewater.

Parameter	Unit	Treated municipal wastewater
pH	–	7.8 ± 0.2
Temperature	°C	19.1 ± 0.1
Conductivity	$\mu\text{S}/\text{cm}$	848 ± 42
Turbidity	NTU	16.8 ± 0.12
Absorbance ($\lambda = 254 \text{ nm}$)	nm	0.196 ± 0.02
COD*	$\text{mg O}_2/\text{l}$	32 ± 4
TOC**	$\text{mg C}/\text{l}$	5.2 ± 0.8
Free chlorine	$\text{mg Cl}_2/\text{l}$	< 0.1 ± 0.03
Iron	mg/l	2.41 ± 0.2
Manganese	mg/l	0.59 ± 0.09
Chloride	mg/l	132 ± 13
Sulfate	mg/l	103 ± 10

* Chemical Oxygen Demand.

** Total Organic Carbon.

Number of samples: three samples mixed together, from which the average value has been obtained, according to [56].

Table 2
Design parameters of the tested wastewater for the modeling process.

Parameter	Unit	Design value
pH	–	7.8
Temperature	K	292.25 ± 273.15
Turbidity	NTU	16.8
Total Suspended Solids	mg/dm ³	25
TOC	mg/dm ³	5.2 ± 0.8
NH ₄ ⁺	mg/dm ³	0.020
K ⁺	mg/dm ³	14.9
Na ⁺	mg/dm ³	120
Mg ²⁺	mg/dm ³	10
Ca ²⁺	mg/dm ³	55.1
Sr ²⁺	mg/dm ³	0.019
Ba ²⁺	mg/dm ³	0.019
CO ₃ ²⁻	mg/dm ³	0.630
HCO ₃ ⁻	mg/dm ³	123
NO ₃ ⁻	mg/dm ³	13
Cl ⁻	mg/dm ³	132
F ⁻	mg/dm ³	0.13
SO ₄ ²⁻	mg/dm ³	103
Br ⁻	mg/dm ³	0.020
PO ₄ ³⁻	mg/dm ³	2.5
CO ₂	mg/dm ³	2.573
Conductivity *	µS/cm	968.93

* value corrected and calculated in the WAVE software.

the tested treated municipal wastewater samples was 848 µS/cm, therefore reverse osmosis was selected as the final process for water production for electrolysis (Table 3). Both 1- and 2-pass processes were analyzed among the selected processing systems. Pre-treatment of the wastewater is required to prepare it for deionization. The membrane filters for RO are exposed to contamination by numerous substances, including natural organic matter, solids, colloids, bacteria, viruses, etc. The above pollutants can be removed by conventional treatment processes consisting of coagulation followed by filtration (for media with low turbidity and total suspended solids – coagulants are added before filter bed entry). In the case of media with high turbidity and total suspended solids, additional stages of sedimentation are carried out before filtering the water/waste. Ultrafiltration is used with alternative pre-treatment methods (primarily for removing turbidity, suspended solids, and bacteria). In the case of membranes for reverse osmosis, antiscalant is dosed in as an addition to minimize the content of calcium carbonate and sulfates to prevent scale sedimentation (membrane fouling). Additional operations may include e.g. water chlorination or UV sterilization (eliminating bacterial flora responsible for biofouling), pH correction, free chlorine reduction, and degassing (CO₂ removal).

It was assumed that the municipal wastewater pre-treatment installation would comprise the following elements: sieve filter, ultrafiltration, and reverse osmosis.

The sieve filter is a pipeline filtering equipment element that can be applied in various branches of industry to fulfill several filtration requirements. The filter insert is located in a casing and is intended to remove solids. The sieve filter's primary purpose is the mechanical protection of downstream devices. The sieve filter offers a filtration accuracy of 100–150 µm. Using ultrafiltration in wastewater treatment typically involves the removal of various suspended solids and dissolved

Table 3
Deionized water production methods.

Wastewater quality	Required water quality	Recommended technology
< 500 µS/cm	< 5 µS/cm	Ion exchange
	< 1 µS/cm	Ion exchange and mixed bed
500–2000 µS/cm	5–20 µS/cm	Reverse osmosis
	< 5 µS/cm	2-pass reverse osmosis
	< 1 µS/cm	2-pass reverse osmosis combined with ion exchange and mixed bed

organic matter with high molecular mass, usually > 5–10 nm [59], as a result of separation by sieving. UF occurs at a pressure of 0.5 to 10 bar. A standard UF installation is typically composed of several sections, comprising: water intake and pressure pumps, initial water preparation, ultrafiltration modules, backwashing, chemical treatment, and water conditioning [60,61]. Reverse osmosis makes it possible to remove very small pollutant molecules from a solution, which concerns particularly monovalent ions. Reverse osmosis is used for water treatment and to remove salts and other pollutants to improve the color, taste, and other properties of liquids. The process makes it possible to remove bacteria, salts, sugars, proteins, dyes, and micropollutants. The RO membrane molecular weight cutoff is < 200 Da. The applied pressure ranges from 3.4 bar to 100 bar. The separation mechanism in reverse osmosis is described by the solution-diffusion model. The model assumes that the flow of specific components through the compact polymer membranes is determined by their solution in the polymer and by diffusion. The model omits the interactions between the membrane polymer and the diffusing component. The components undergo diffusion through the membrane under the influence of a thermodynamic impulse, i.e. the negative gradient of that component's chemical potential. However, reverse osmosis is significantly different from other techniques of this type, such as ultra- and microfiltration. In RO processes, solution and diffusion constitute the basic separation mechanism, whereas the sieving effect does not occur at all [62,63].

2.3.3. Modeling a membrane filtration process

The membrane filtration process modeling was conducted using the WAVE (Water Application Value Engine) software by DuPont (version 1.82.824). The WAVE software is intended for designing and simulating the operation of treatment systems involving membrane filtration. WAVE is an integrated software for expert modeling, developed for designing treatment plants, including wastewater treatment plants. The program combines leading membrane technologies: ultrafiltration (UF), reverse osmosis (RO), and ion exchange (IE), into a single, comprehensive platform. The WAVE software is based on the diffusion model and integrates the model's equations to simulate the flow of molecules through a semi-permeable membrane, and it is used to design and simulate the operation of water treatment systems involving UF, RO, and IE as constituent processes [64,65]. An attempt was undertaken to design a reverse osmosis installation for treated municipal wastewater deionization to use the wastewater as a feedstock for electrolysis. A computer simulation was carried out to verify the desired conductivity of < 5 µS/cm. Seven processing cases were subjected to analysis (Table 4).

The conductivity of the filtrate after UF/RO, which determines the applicability of the reclaimed water in the electrolysis process (max. 5 µS/cm), was the most crucial parameter on which modeling was focused. This work also involves the study of the factors determining: (a) operating costs (electricity consumption); (b) operating costs and injection of reagents (pH of the filtrate); and (c) operating costs and the negative phenomenon of limescale deposition on equipment and thus reducing the efficiency of hydrogen production (cation and anion concentration, including calcium, magnesium, and sulphate). The ultrafiltration process in all case studies was adopted to remove suspended solids and microorganisms. The elimination of suspended solids is designed to reduce the phenomenon of membrane fouling (membrane blockage due to the accumulation of contaminants on the membrane surface and inside the pores) and to protect the equipment from mechanical damage. The elimination of microorganisms is designed to reduce biofouling, i.e. biofilm growth over the membranes, which also reduces membrane permeability. For a flow rate of 133–145 m³/h, the use of 4 working UF trains and two redundant trains was adopted. UF and RO design parameters are derived from membrane suppliers' guidelines and literature data [66–70]. The 1-pass RO was adopted to test the efficiency of ion removal on a simplified technology scheme, as well as the possibility of reducing the investment and operating costs of

Table 4
Types of technological variants for membrane filtration.

Parameter	Unit	Case I	Case II	Case III	Case IV	Case V	Case VI		Case VII	
							Pass 1	Pass 2	Pass 1	Pass 2
ULTRAFILTRATION										
Feed (Wastewater) flow to UF	m ³ /h	133.3	137	137	133.3	133.3	145.4		145.4	
Permeate (product) flow	m ³ /h	100								
Type of membranes	–	Ultrafiltration SFP-2880								
Number of trains (working)	–	4								
Redundant trains	–	2								
Recovery	%	98								
TOC rejection	%	10								
REVERSE OSMOSIS										
Feed (Wastewater) flow to RO	m ³ /h	133.3	137	137	133.3	133.3	145.4	109	145.4	109
Number of passes	–	1	1	1	1	1	2		2	
Number of stages	–	1	2	1	2	2	1	1	2	2
Recovery	%	75	81.1	75	81.3	84.1	68.8		68.8	
Type of membranes	–	SW30XLE-400i								
Active area	m ²	37.2								
Pressure	bar	55.2								
Flow	m ³ /d	34.1								
Rejection	% NaCl	99.8								
Pressure vessel per stage (stage 1 / stage 2)	–	36 / 0	36 / 1	36 / 0	36 / 1	50 / 10	26	26	26 / 1	26 / 1
Elements per pressure vessel	–	6 / 0	6 / 6	6 / 0	6 / 6	6 / 6	6	6	6 / 6	6 / 6
Total elements	–	216 / 0	216 / 6	216 / 0	216 / 6	300 / 60	156	156	156 / 6	156 / 6
Flux	dm ³ /m ² × h	12.5	12.1	12.5	12.1	8.8	18.1	16.6	18.1	16.6
Concentrate recycle	%	0	10	10	0	0	0	0	0	0

the technology. However, since the demineralization technology guidelines show that a 2-pass RO system is recommended to achieve conductivity < 5 us/cm, for this purpose this system was used to validate the data reported in the literature. The number of pressure vessels and elements per vessel was derived from the minimum and maximum recommended values of concentrate flow and recovery per element for a given membrane type, as determined by the WAVE program (based on the supplier's guidelines). The concentrate recirculation was assumed at a maximum of 10 % in order to adjust the minimum or maximum flow rate according to the membrane manufacturer's instructions. The selection of power was based on the assumed capacity, flow and heading head (geometric height, losses). In all cases, it was determined that the treated wastewater would be taken from an intermediate tank located at a distance of up to max. 10 m from the membrane installation. The parameters given in the Table 4, such as feed flow, flux, recovery rate, active area, TOC and salts rejection, etc., result from the assumed initial parameters and parameters determined by the membrane properties.

The data presented in this article is important because it allows verification and validation of the performance of the designed treatment system. The data presented is also significant because it allows to verify the assumed requirements for the quality of reclaimed water, the adopted design or operational parameters. With a very large number of parameters that can affect the final efficiency of the electrolyzer, the proper selection of a technological system for the recovery of water from municipal wastewater, which is a mix of different substances, it is often necessary to adapt a specific solution to a particular wastewater stream, which makes it very difficult to develop a uniform technological system for the water recovery as an input for the electrolyzer. To simplify the problem, the data presented in this article take into account the most important requirements for the quality of the electrolyzer feedwater to provide sufficiently low conductivity of reclaimed water and make the concentrations of problematic ions certainly lower than the requirements of electrolyzer manufacturers. To provide design support for this framework, the data presented allows for the modeling and computational analysis of membrane systems through their unique features and parameters, based on actual input data from a real municipal wastewater effluent.

3. Results and discussion

As part of the first case, the analysis involved a process comprising membrane filtration on membranes for ultrafiltration and reverse osmosis (Fig. 1). The processing system included 1-pass RO with 1-stage membrane filtration. The 1-stage filtration involved 36 pressure vessels, with 6 elements per vessel. The calculated flux was 12.5 dm³/m² × h (flow per unit of membrane surface). A pump with a power of 38.7 kW was proposed. The theoretical total energy consumption was about 929.5 kWh/d. The total water recovery was 75 %.

Fig. 2 presents the proposed design solution of the case II membrane filtration system, i.e. a processing system composed of 1-pass RO with 2-stage membrane filtration. The 1-stage filtration involved 36 pressure vessels, with 6 elements per vessel. The 2-stage filtration involved 1 pressure vessel, with 6 elements in the vessel. The calculated flux was 12.1 dm³/m² × h. A pump with a power of 36.2 kW was proposed. The theoretical total energy consumption was about 867.7 kWh/d. The total water recovery was 81.3 %.

Case III involved a membrane filtration system comprising UF and RO as part of a 1-pass RO system with 1-stage membrane filtration (Fig. 3). This case included a concentrate recycle to the membrane system entry to an amount of 3.7 m³/h (10 % of feed flow). Depending on the applied membrane types, concentrate flow modeling enables the adjustment of the minimum or maximum flow as per the membrane manufacturer's instructions. However, due to concentration, the water recovery decreases over subsequent passes (to about 73 %), and the net recovery equals 75 %. As a result of concentration, the water reclaimed from wastewater is also characterized by higher conductivity. In the first stage, the reclaimed water conductivity was 9 µS/cm, while in the second it was 48 µS/cm. The final calculated concentrate conductivity was 10 µS/cm. A pump with a power of 38.7 kW was proposed. The theoretical total energy consumption was about 929.5 kWh/d.

Case studies IV and V involved the analysis of two processing systems comprising 1-pass RO with 1-stage membrane filtration. The differences between the two analyzed cases consisted of the different total number of applied pressure vessels. A total of 212 vessels and 360 vessels was proposed for case study IV and V respectively (Fig. 4). The number of pressure vessels reduces the permeate flux – the greater it is, the lower the flux and the greater the recovery, with the simultaneous minor deterioration of the water quality. For case study IV, the recovery was

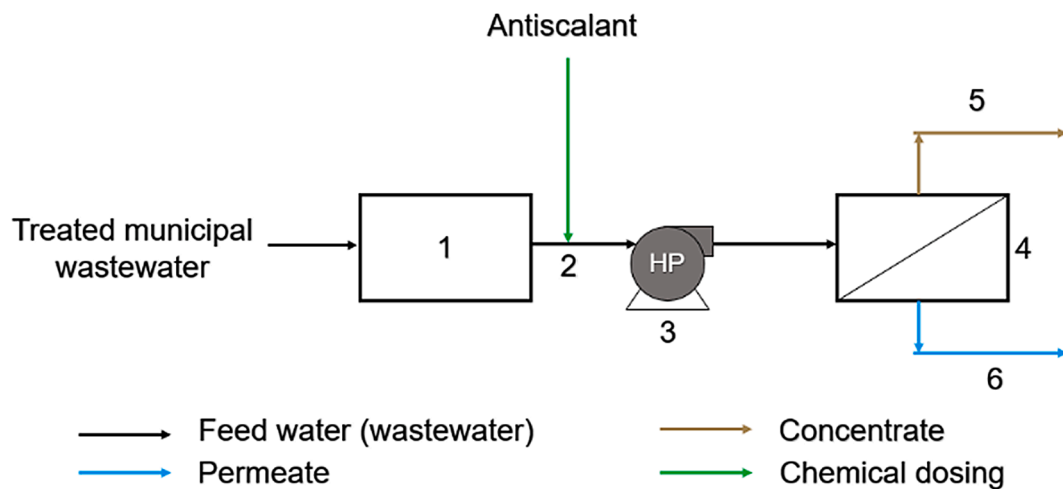


Fig. 1. Process flow – Case I 1 – Ultrafiltration unit; 2 – Antiscalant dosing; 3 – Pressure pump; 4 – 1-pass, 1-stage RO unit; 5 – Final concentrate; 6 – Permeate.

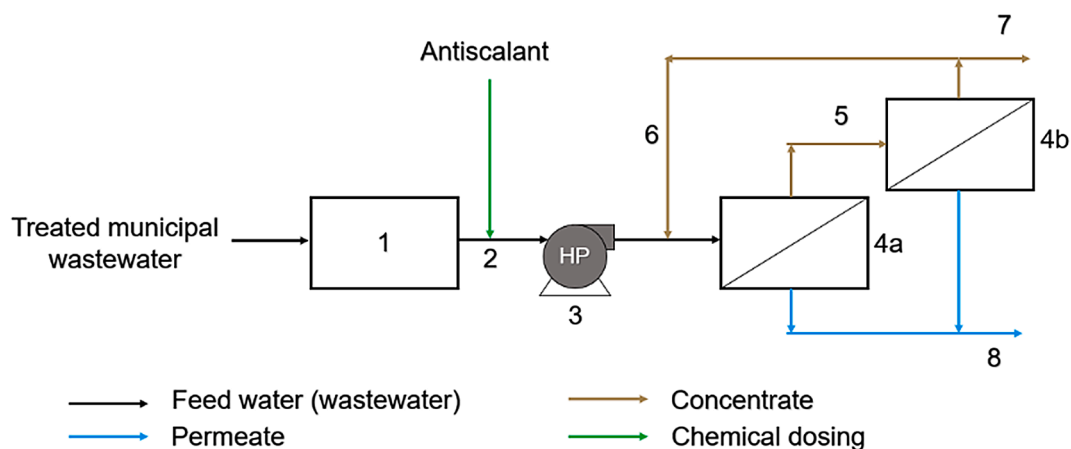


Fig. 2. Process flow – Case II 1 – Ultrafiltration unit; 2 – Antiscalant dosing; 3 – Pressure pump; 4a – 1-pass, 1-stage RO unit; 4b – 1-pass, 2-stage RO unit, 5 – Concentrate from 1-stage RO unit; 6 – Concentrate recycle; 7 – Final concentrate; 8 – Permeate.

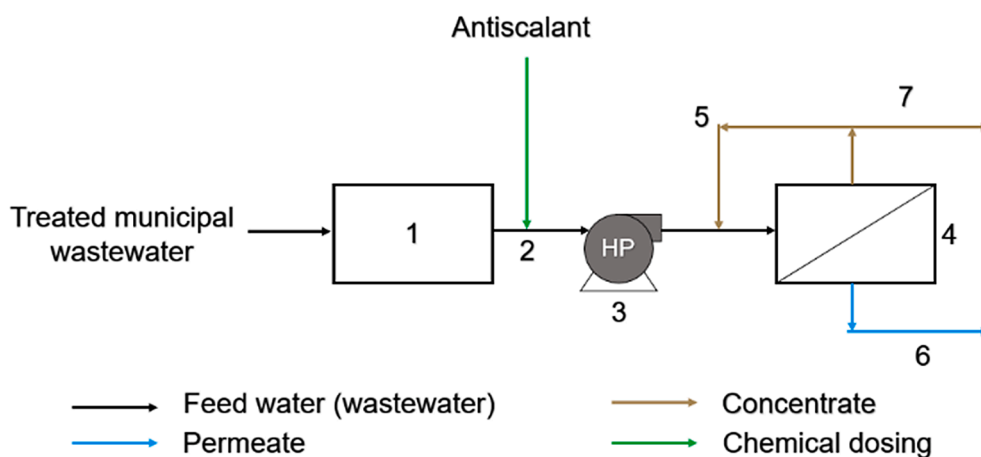


Fig. 3. Process flow – Case III 1 – Ultrafiltration unit; 2 – Antiscalant dosing; 3 – Pressure pump; 4 – 1-pass, 1-stage RO unit; 5 – Concentrate recycle; 6 – Permeate; 7 – Final concentrate.

81.3 % at a final calculated average conductivity of 10 $\mu\text{S}/\text{cm}$, whereas for case study V the values were 84.2 % and 13 $\mu\text{S}/\text{cm}$ respectively. The installation proposed as part of case study V was characterized by the lowest energy consumption (about 606.1 kWh/d) due to the application of pumps with lower power and a higher number of pressure vessels.

However, considering the unsatisfactory quality of the permeate, this processing system is not recommended.

For cases VI and VII, the proposed processing system comprised 2-pass membrane filtration. Case VI encompassed the application of 1-stage reverse osmosis as part of each pass (Fig. 5). Case VII was

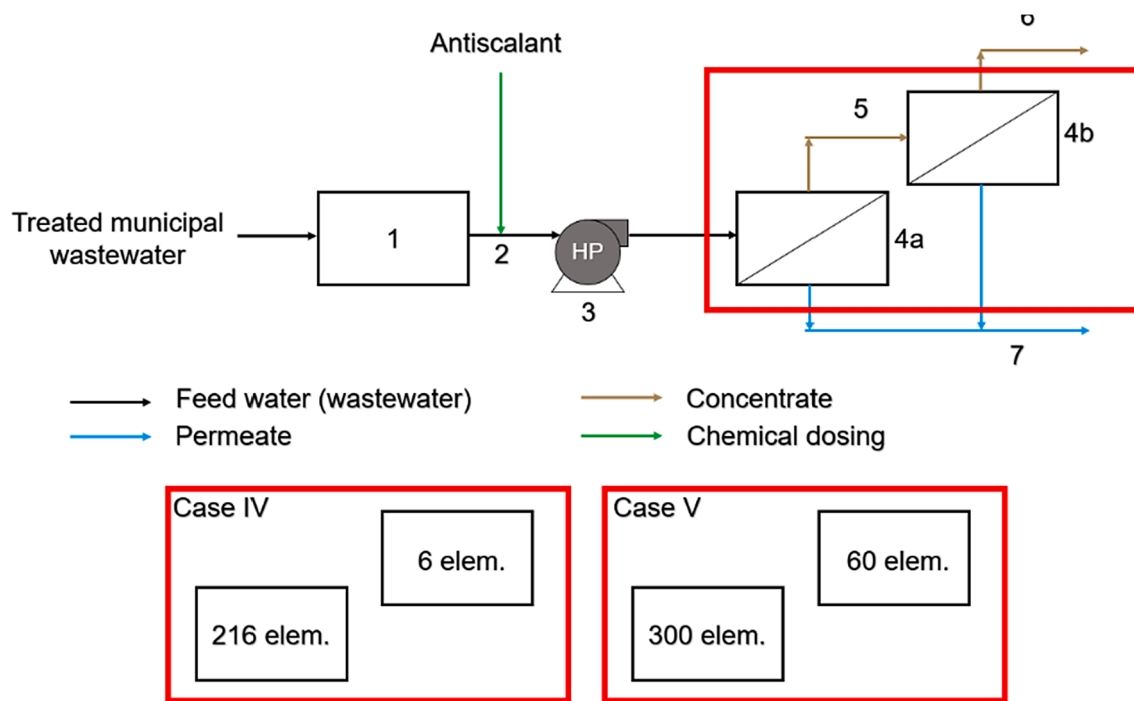


Fig. 4. Process flow – Case IV and Case V 1 – Ultrafiltration unit; 2 – Antiscalant dosing; 3 – Pressure pump; 4a – 1-pass, 1-stage RO unit; 4b – 1-pass, 2-stage RO unit, 5 – Concentrate from 1-stage RO unit; 6 – Final concentrate; 7 – Permeate.

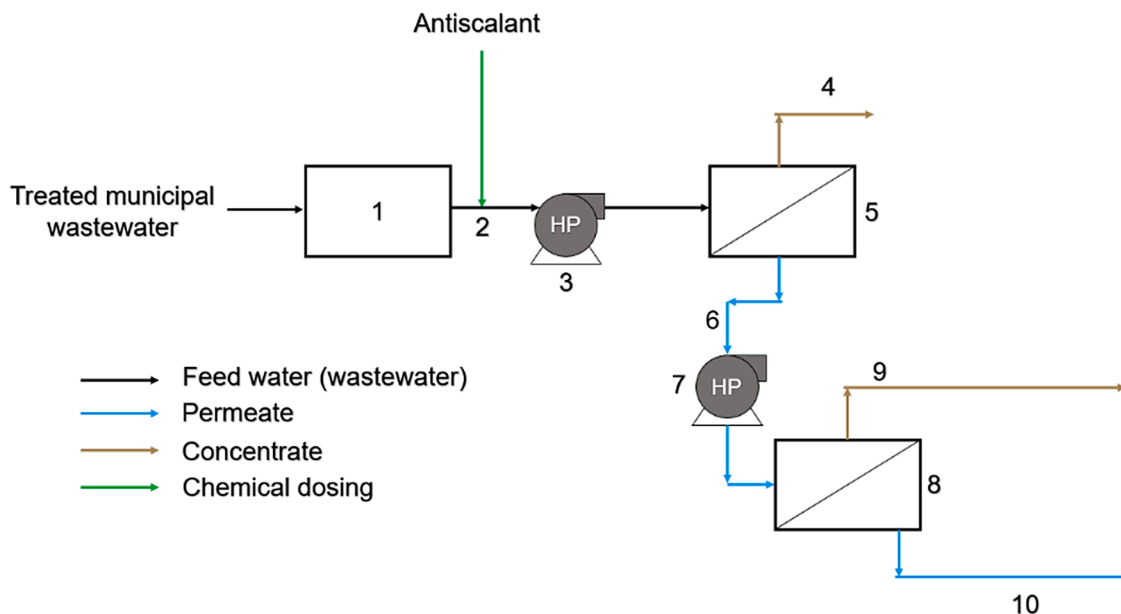


Fig. 5. Process flow – Case VI 1 – Ultrafiltration unit; 2 – Antiscalant dosing; 3, 7 – Pressure pump; 4 – Concentrate from 1-pass, 1-stage RO unit; 5 – 1-pass, 1-stage RO unit; 6 – Permeate from 1-pass, 1-stage RO unit; 8 – 2-pass, 1-stage RO unit; 9 – Concentrate from 2-pass, 1-stage RO unit; 10 – Final permeate.

expanded by 2-stage membrane filtration as part of each 2-pass process (Fig. 6). The net water recovery was similar in both cases and amounted to 68.8–71.8 %. In both cases, the application of 2-pass reverse osmosis made it possible to recover water with an average calculated conductivity of 2 $\mu\text{S}/\text{cm}$. Taking into account the conformity with the design assumptions, cases VI and VII are the recommended systems for water recovery from the analyzed municipal wastewater.

Fig. 7 shows a compilation of the conductivity of water reclaimed from municipal wastewater treated as part of the analyzed processing systems. The conductivity (an electrical conductivity of water) is defined as the capacity of the water to transmit a flow of electricity (to carry an

electrical current) [71]. The electrical conductivity of water is affected by the presence of ions that carry a negative and positive charge such as chlorides, sulphates, calcium, and magnesium [72]. As can be observed from the presented data, case VI and case VII make it possible to obtain deionized water with parameters fulfilling the requirements for electrolyzer feedstock (water conductivity < 5 $\mu\text{S}/\text{cm}$). The proposed solutions can yield about 100 m^3/h of deionized water with a conductivity of about 2 $\mu\text{S}/\text{cm}$ over 1 h of operation. Obtaining the intended product efficiency requires about 133 to 145 m^3/h of treated municipal wastewater. Low conductivity is important for several reasons. First, the higher the content of undesirable ions, the more the composition of the

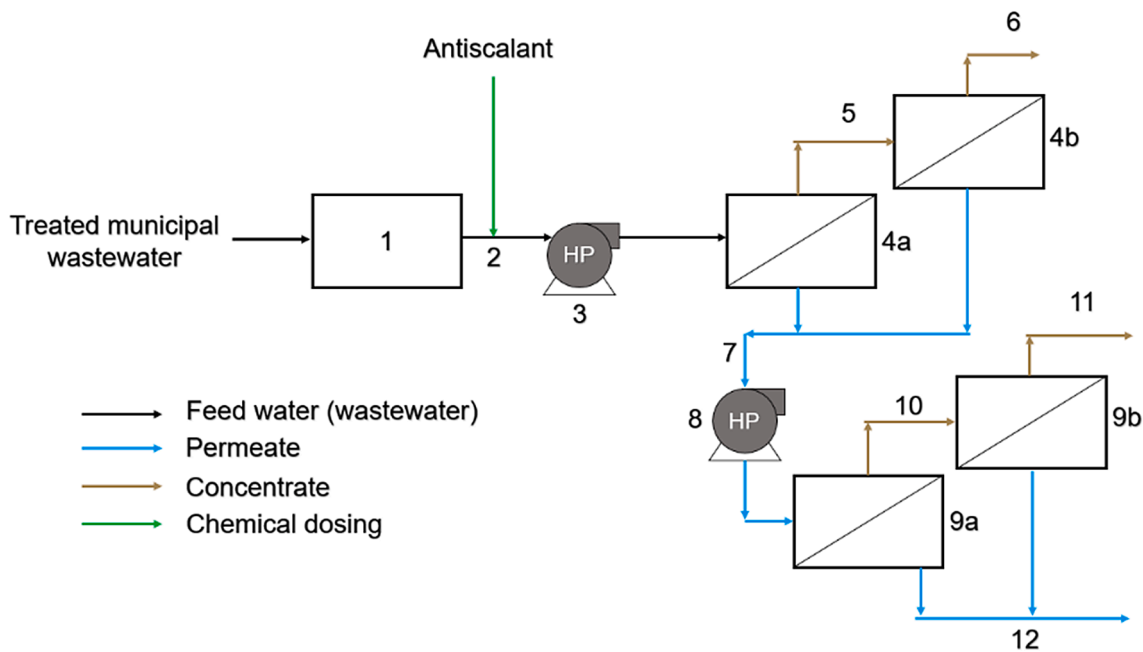


Fig. 6. Process flow – Case VII 1 – Ultrafiltration unit; 2 – Antiscalant dosing; 3, 8 – Pressure pump; 4a – 1-pass, 1-stage RO unit; 4b – 1-pass, 2-stage RO unit; 5 – Concentrate from 1-pass, 1-stage RO unit; 6 – Concentrate from 1-pass, 2-stage RO unit; 7 – Permeate from 1-pass RO units; 9a – 2-pass, 1-stage RO unit; 9b – 2-pass, 2-stage RO unit; 10 – Concentrate from 2-pass, 1-stage RO unit; 11 – Concentrate from 2-pass, 2-stage RO unit; 12 – Final permeate.

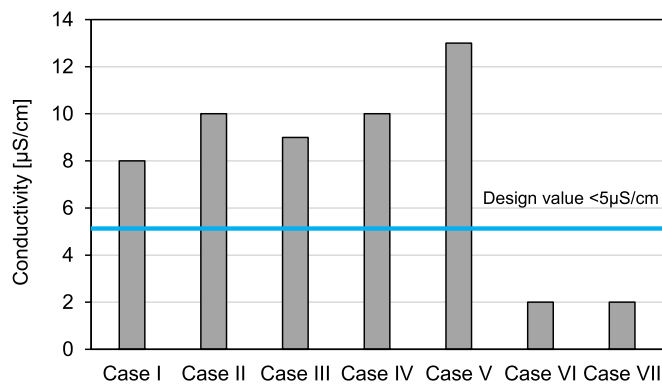


Fig. 7. Summary of conductivity values for each case study.

extracted gas changes. Due to the undesirable components contained in poorly treated water, the composition of the gas is changing. This low conductivity avoids interference of signals by ions in the water. Ions in the feed water can also interact with the electrolyzer material, which can lead to changes in electrical properties and affect results. Since municipal wastewater (even treated wastewater) is a mix of different types of substances, municipal wastewater presents technical and technological

challenges to make it possible to produce ultra-pure hydrogen (purity of $\geq 99.999\%$). Furthermore, maintaining a low conductivity (and thus a low content of undesirable ions) is expected to prevent equipment corrosion and biofouling of the electrolyzer. High water conductivity also has a major impact on the lifetime of the electrolyzer, which can in turn affect hydrogen cost by increasing the annuity of the electrolyser in the cost of hydrogen [73-77].

Table 5 presents a compilation of the analyzed case studies with the most important membrane filtration modeling results obtained. The output filtrate production (water after UF/RO) was set at $100\text{ m}^3/\text{h}$ for all cases. The water recovery rate ranged from about 69 % to up to 81 % at an effluent inflow rate of about $133\text{ m}^3/\text{h}$ to $145\text{ m}^3/\text{h}$, depending on concentrate recirculation. The results obtained based on an analysis of 7 different processing cases studies (ultrafiltration and reverse osmosis) confirmed that the application of 2-pass membrane systems enables the reclamation of water from municipal wastewater that fulfills the requirements concerning the quality of water intended as electrolyzer feedstock, as the obtained water exhibited a conductivity of $< 5\text{ }\mu\text{S}/\text{cm}$. Depending on the analyzed case study, the attainable level of water reclamation ranged from 68.8 to 84.1 % at an energy consumption of 606.1 – 2 694 kWh/d. The results of this work not only confirm that the selected processing solutions make it possible to reclaim water from municipal wastewater, but also confirm the necessity of using software

Table 5
Specific parameters for the analyzed case studies.

Parameter	Unit	Case I	Case II	Case III	Case IV	Case V	Case VI	Case VII
Feed wastewater	m^3/h	133.3	137	137	133.3	133.3	145.4	145.4
Produced water	m^3/h	100	100	100	100	100	100	100
Recovery	%	75	81.1	75	81.3	84.1	68.8	68.8
Conductivity	$\mu\text{S}/\text{cm}$	8	10	9	10	13	2	2
Permeate TDS	mg/dm^3	4.97	6.34	4.97	5.84	7.77	3.33	3.70
Mg^{2+}	mg/dm^3	0.02	0.02	0.02	0.02	0.02	0.01	0.01
Ca^{2+}	mg/dm^3	0.08	0.10	0.08	0.10	0.12	0.05	0.06
Cl^-	mg/dm^3	0.82	1.06	0.82	0.97	1.33	0.53	0.60
SO_4^{2-}	mg/dm^3	0.08	0.10	0.08	0.09	0.12	0.05	0.06
pH	–	5.8	5.9	5.8	5.9	6.0	5.7	5.7
Energy consumption	kWh/d	929.5	867.7	929.5	858.4	606.1	2694	2569

to simulate the membrane system operation to select the most economic and cost-effective solution. The pH of the demineralized water would also need to be factored in when selecting the appropriate processing system. The reaction of the obtained water did not exceed $\text{pH} = 6$ for all the analyzed cases. After demineralization, the process water should be conditioned according to the electrolyzer manufacturer's specifications and the process water requirements. For example, the pH of the feed water to the HySTAT electrolyzers [78] should be between 5.0 and 7.0 (information obtained from the electrolyzers' supplier), so each of the streams recovered from the wastewater meets this parameter.

Furthermore, defining the optimal processing system should also factor in the risk of membrane scaling. WAVE does not provide a mechanism for estimating the antiscalant efficiency, therefore the choice of both the antiscalant and its dosage as well as its efficiency should be investigated accordingly and determined at the stage of technology selection. As presented above, among the 7 analyzed processing systems, only cases VI and VII exhibit a quality of the reclaimed water compliant with ASTM's requirements. Considering the high efficiency and the expanded processing system structure, energy consumption in these cases is higher compared to the others, but these cases exhibit the best water quality. Both the analyzed cases are characterized by similar power demands, but the energy consumption for case VII is nearly 5 % lower relative to the energy consumption for case VI at almost equivalent reclaimed water quality, therefore case VII appears to be the optimal solution from this perspective. Assuming a water consumption of 15 kg H₂O/ 1 kg H₂ for electrolysis (factoring in water loss for rinsing and cleaning as well as an electrolyzer efficiency of about 60 % [48]), at the adopted installation efficiency, the hydrogen yield over 1 h would equal about 6666 kg H₂.

In the study case appearing as the optimal (case VII), the doubtless advantages of the process include the lack of chemical dosing, since the operation of the system relies only on pressure as the driving force, and the separation takes place at room temperature, with no phase change. The proposed technology can even function as a stand-alone process system, compared, for example, to distillation which is currently not cost-effective due to high energy consumption, when used as a single reclaiming technology. Compared to distillation or evaporation processes, as the methods for wastewater treatment and water reclamation, the proposed technology is highly competitive in terms of electrical consumption (1.07 kWh/m³). Classical distillation or evaporation technologies, in addition to the electrical energy requirements (approx. 0.5 to 5.0 kWh/m³), also involve a thermal energy consumption (approx. 27–83 kWh/m³) [79-81]. Although 2-pass RO is an effective method for water reclamation, as all membrane processes has certain limitations, such as the phenomenon of membrane fouling, which forces the need for frequent membrane flushing or dosing of cleaning chemicals. The RO process also produces an additional stream of waste liquid (concentrate), which must be eliminated. Due to the recovery rate (68–84 %) of water, the RO process also produces an additional stream of waste liquid (concentrate), which must be eliminated.

Compilations of the estimated investment and operating costs are presented in Table 6 and Table 7 respectively. The appropriate indices recommended for flow processes were applied to evaluate the investment and operating costs [82-84]. The data pertains to a processing system with an efficiency of 100 m³/h of the product (water reclaimed from municipal wastewater). Direct costs (D) include the costs of purchasing equipment and machinery (E), as well as instrumentation, control systems, pipelines, electric systems, land improvement, wastewater treatment plant operation adjustments, buildings, maintenance equipment (D1), etc. The costs of equipment and machinery were adopted based on information obtained from suppliers, analyses, and own experience. Indirect costs (I) include aspects such as technical design costs and legal expenses. The economic analysis also encompasses certain risk factors and the costs of unforeseen events. The annual operating costs encompass chemicals, media, manpower, maintenance, and insurance. To calculate the annual costs, the analysis assumed the

Table 6
Estimated capital costs.

Parameter	Factor	Estimated Cost [US\$]
Equipment and devices (E)	-*	650,000
Other capital cost (D1)		
-Electrical	25 % x E	162,500
-Piping	10 % x E	65,000
-Installation	35 % x E	227,500
-Instrumentation and control	15 % x E	97,500
-Land improvement	1 % x E	6,500
-WWTP improvement	50 % x E	325,000
-Building cost	15 % x E	97,500
Other capital cost (D1)		981,500
Total direct cost (D)		1,631,500
Technical design	15 % x D	244,725
Engineering	20 % x D	326,300
Legal expenses	4 % x D	65,260
Total indirect cost (I)		636,285
Direct and indirect cost (D + I)		2,267,785
Contractor fees	5 % x (D + I)	113,389
Unforeseen expenses	10 % x (D + I)	226,779
Total investment cost		2,607,953

* Based on suppliers' information, own analyses and experience from similar implementations.

Table 7
Estimated annual operating costs.

Parameter	Factor	Estimated Cost [US\$/year]
Concentrate disposal	-*	131,900
Electricity	-*	177,217
Chemical dosing	-*	26,285
Workers (W)	2 × 1100 US\$/month	26,400
Insurance	2 % x E (Table 6)	13,000
Maintenance (M)		
-Mechanical	7 % x E (Table 6)	81,575
-Civil	3 % x D	48,945
Supervisor	25 % x W	6,600
Laboratory	10 % x W	2,640
Repairs	40 % x M	52,208
TOTAL OPERATING COSTS		566,769

* Based on WAVE calculations.

employment of 2 workers and an installation operation of about 363 days per year, factoring in technical pauses of about 4 h a month. The total investment costs for an installation with an efficiency of 100 m³/h may amount to an average of about US\$2,206,729. Meanwhile, the costs of operation and maintenance may amount to an average of about US\$536,657, factoring in the costs of concentrate management and disposal after RO.

4. Conclusions

- The paper presented an analysis of selected processing systems comprised of 1- or 2-pass membrane processes (ultrafiltration and reverse osmosis).
- Commercial software for selecting membrane modules, provided by their producers, is very useful in the process of designing the appropriate membrane system. Modeling the membrane filtration process for water reclamation from municipal wastewater to produce water intended as a feedstock for electrolyzers was conducted using the DuPont Water Solutions WAVE software for the actual conditions and parameters of a functioning public utility facility – a wastewater treatment plant with a population equivalent (PE) of > 100,000.
- 7 processing cases for treated municipal wastewater deionization were proposed to use the water as a feedstock for electrolysis, and a computer simulation was carried out to determine the desired conductivity of < 5 μS/cm. It was assumed that the municipal

wastewater pre-treatment installation would comprise the following elements: sieve filtration, ultrafiltration, and reverse osmosis.

- Two of the 7 processing cases made it possible to recover water of the expected quality (case VI and case VII). The obtained data also confirms that the instructions of membrane manufacturers in terms of technology selection were fulfilled. The analyzed 1-pass systems failed to yield water with parameters enabling its use as an electrolyzer feedstock. On the other hand, the analyzed 2-pass systems made it possible to recover water exhibiting a conductivity fulfilling the requirements of ASTM, i.e. water with a conductivity of < 5 µS/cm.
- Both the analyzed cases were characterized by nearly identical compositions of the permeate (water reclaimed from wastewater) and similar demands for electric power, though case VII exhibited a lower energy consumption. From this perspective, case VII was proposed as the recommended solution, though the final choice between cases VI and VII require more in-depth consideration, as the membrane with the highest efficiency also exhibited the highest power demand. In this regard, cost factors play a greater role.
- The work conducted as part of this paper confirmed the possibility of reclaiming water from municipal wastewater. The recovery of water with parameters fulfilling the requirements for electrolyzer feedstock was confirmed based on the modeling results.
- This work confirmed the necessity of utilizing software to simulate the operation of membrane systems to select the most economic and cost-effective solution.

Funding sources

The presented study was performed as part of the research work of the Central Mining Institute in Poland, with financial support by the Polish Ministry of Science and Higher Education [No. 11131032-340].

CRedit authorship contribution statement

Piotr Zawadzki: Conceptualization, Methodology, Investigation, Writing – original draft, Software, Data curation. **Beata Kończak:** Conceptualization, Methodology, Supervision, Writing – review & editing. **Adam Smoliński:** Conceptualization, Methodology, Supervision, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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