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Review

Optimization of MBRs through integrated modelling: A state of the art

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A B S T R A C T

The optimization of integrated membrane bioreactors (MBRs) models is of paramount importance in view of reducing the costs, greenhouse gas emissions or enhancing the water quality. On this behalf, this paper, produced by the International Water Association (IWA) Task Group on Membrane modelling and control, reviews the current state-of-the-art regarding the control and optimization of integrated MBR models. Whether aerobic or anaerobic, such modelling allows the consideration of specific functioning conditions and optimization problems together with the estimation and monitoring of Performance Index (PIs). This paper reviews the diversity of those problems criteria used in performance assessment. Dividing issues that can be addressed either off-line or online, it is shown that integrated models have attained an important degree of maturity. Several recommendations for mainstreaming the optimization of MBRs using such integrated models. The key findings of this work show that there is room for improving and optimizing the functioning of MBRs using integrated modelling and that this integrated modelling approach is necessary to link functioning conditions together with PI estimation and monitoring.

1. Introduction

When dealing with wastewater treatment processes, membrane bioreactors (MBRs) are excellent candidates since they allow almost any quality level of treated water while guaranteeing health and environmental safety. An MBR is a very efficient water treatment with several advantages over conventional technologies. Maintaining a pressure difference on both sides of the membrane creates a driving force for the fluid to be treated, enabling the separation of the various solutes present. Depending on the technology used, the membrane may be immersed or external. MBRs are used for municipal and industrial wastewater treatment applications (Judd and Judd, 2011). However, such systems still suffer from relatively high capital expenditures (CAPEX) and operating expenses (OPEX), and membrane fouling remains one of the main problems. The optimization of an MBR plant is a challenging task due to numerous specific conditions concerning its functioning (Krzeminski et al., 2017).

An MBR usually operates in alternating filtration and backwash/relaxation phases. Often, it is also submitted to varying inputs: it is thus a complex "dynamical system", the optimization of which has attracted much attention these last years. It refers to the search for optimal trajectories – concerning a given criterion or set of criteria - by manipulating several degrees of freedom (named control variables in a dynamical context), possibly under several constraints specified by the user. This very general definition calls for several important remarks.

First, in the static case (when time is not considered), an optimization is nothing more than finding the minima or maxima of some function (i.e., the optimization criterion). Then, in a model identification procedure, these values of model parameters – or control inputs and setpoints - are to be identified. At the same time, the optimization criterion is a measure of the distance between the available data and model predictions. In a "design optimization problem" (i.e. finding the best values of a given process input, for instance), the problem often reduces to the capacity of the user to explore a grid of values for this degree of

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freedom and to retain that one which minimizes/maximizes the cost function, if the parameter space (i.e. the number of degrees of freedom) is very small. In the dynamic case (i.e. finding the best trajectory of a control input/setpoint/free parameter), it is no longer a single value searched for. Still, precisely a trajectory - otherwise, an infinite number of values! In addition, notice that even in an academic example where the parameter and state spaces would be very small, the "capacity to experiment" may take a very long time when confronted with a fundamental process optimization problem. Indeed, solving a dynamical optimization problem is a difficult task. In the presence of nonlinearity (either in the criterion, which is sometimes the case with the issues of interest here or in the system, which is always the case in the considered MBR models), the uniqueness of the optimal solution is not guaranteed, and, from the best of authors knowledge, there is no guarantee that the computed solution be the global optimum.

When dealing with MBR control and optimization, we are dealing with three major questions.

- The first question to be asked is thus to formalize which criterion to be optimized, i.e., which target must be achieved to reach an optimal operating status and how this target (hereafter named "Performance Index" or PIs) be quantified. To answer this first question, we claim that integrated modelling is a key to correctly proceeding.
- The second question is related to the user's capacity to address MBR optimization questions: is the optimization problem static (for instance, optimize some design parameters such as volumes, recirculation rates, and operating setpoints …) in the presence of constant environmental inputs or dynamic (for example, find the appropriate feedback loops such that disturbance(s) be rejected and while a given (or several) criteria be optimized)? Independently of the optimization method used, the main difference between both questions is the real-time nature - the online implementation - of the second for the first. What can integrated models be used for in these two contexts, and how can they be used? For optimizing the functioning of a system, the optimizer needs "to know" the system and, in particular, how it reacts when the optimization parameter(s) is (are) manipulated. In other words, how the variables that appear in the optimization criterion, which are often the performance indicators we just mentioned, are related to the available model of the process. For MBRs, the "price to pay" is the need for an integrated process model to be optimized. It is often forgotten, but one of the significant advantages of having a dynamic process model is quantifying the distance from the theoretical optimum (assuming it may be found and qualified as such) at which the system operates for any given functioning mode. Applying an integrated approach may thus provide a faster solution to help MBR achieve a more sustainable performance. With this regard, a framework that couples an integrated model with algorithms that correctly estimate performance indicators may become an important analytic tool to pursue better outputs.
- The third question we may ask is to return to the online implementation of process optimization: how can we implement such optimization strategies? This question is somewhat related to implementing online control. The results of optimization procedures - such as those resulting from applying optimal control theory - often do not give any practical information about their online implementation. The rule rather than the exception is that they provide so-called open-loop optimal trajectories but do not provide any feedback structure to apply them in practice. Thus, this third question relates to how we can implement online optimal control solutions for MBRs to optimize their practical functioning. With integrated modelling, this question is addressed in two ways in the literature. Either integrated models are used as a means of simulating a real process - a virtual process - on which optimization strategies are tested following a "plant-wide control" approach: in this family, we find articles dealing with the evaluation of membrane filtration controls just as much as articles dealing with the optimization of the biological functioning of the system. Either integrated model is used to optimize real systems. There are far fewer articles following this logic, as it requires the prior identification of an integrated model to simulate satisfactorily the actual process to be optimized.

In line with the work initiated and realized within the IWA Working Group on MBR modelling these last years, we aim to provide a literature review of MBR optimization and give some insights into their online optimization. While optimization is permanently coupled to modelling, this paper focuses on the optimization part, given that the integrated modelling aspect is addressed elsewhere (Mannina et al., 2021).

The paper is organized around the three important questions that were raised above. In section 2, we express the concept of multi-objective assessment for MBRs. In particular, it is insisted that the performance objectives are no longer captured by a single criterion but rather follow a multi-objective framework. In section 3, we review the literature for each performance indicator. Then, we examine the specificities of MBRs with respect to optimization purposes in a section named "Integrated MBR models towards optimization". Section 4 explains how PIs and integrated modelling must be considered for the optimization problems of interest. Considering that fouling control is one of the main levers of action for the practical improvement of MBR operation, we devote section 5 to a review of approaches enabling its online optimization. Finally, we recommend online optimization of MBRs to improve their performances while minimizing their OPEX and CAPEX. Of course, this paper is related to control and optimization, OPEX is much more addressed than CAPEX. However, searching for the best configuration may have an important influence on CAPEX associated with the number of Pis reviewed (for instance, on the system's volume), as we will see in the following sections.

2. Multi-objective performance assessment

Before optimizing any MBR, it is important to understand which MBR issues may be modelled, i.e., which target must be achieved to reach an optimal operating status, in a sense, to be precise. For example, membrane fouling is one of the most addressed topics among literature reviews related to MBR issues, which is why it may be considered an important target to be optimized. Moreover, this fouling increases energy consumption, which is also another significant target since MBRs are known to consume at least two times more energy than conventional activated sludge systems (CAS) (Bertanza et al., 2017; Cornel and Krause, 2006; Gil et al., 2010), mainly due to the high aeration demand (Sun et al., 2016). Regarding aeration, within an MBR system, this feature has two main goals, often through two different aeration devices: preventing membrane fouling due to the capability of acting over the cake layer (Meng et al., 2019; Du et al., 2019) and enhancing biological performance due to its positive effects over nitrification (Yang et al., 2016; Zheng et al., 2018). This aeration demand is also linked to the TSS concentration, which impacts the reactor design (volume). Considering that these two purposes are highly relevant to the plant's performance, one may consider aeration an important target to optimize.

Effluent quality is another target that may be considered whilst seeking the optimization of an MBR plant since it provides the highest attainable performance for a biological process and the highest effluent quality with more reuse and disinfection capabilities when compared to CAS (Judd and Judd, 2011; Hamedi et al., 2019). Bertanza et al. (2011) also demonstrated a higher ability to reduce the estrogenic activity of the effluent. GHG emissions may also be assessed since MBRs are known to emit the three major gases that represent GHGs: carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O). These emissions can be direct (i.e., from biological processes) or indirect (i.e., from electricity and chemical consumption) (Bao et al., 2016; Parravicini et al., 2016; Pol-ruang et al., 2018). In particular, MBR is accounted for indirectly emitting more CO_2 than CAS due to the high energy. Finally, MBR's high-cost demand is considered one of the major drawbacks of the scattering of the technology, which is why the operating cost can be regarded as one of the most critical targets when assessing MBR's optimization.

As mentioned above, effluent quality, membrane fouling, operating costs, GHG emissions, aeration and energy consumption are targets to be achieved while managing an MBR to optimize its functioning. Thus, considering these six targets provides a framework for MBR optimization related to plant performance. However, building a connection between the integrated MBR model and the targets is important to become quantifiable and, consequently, optimizable. In this regard, establishing performance indicators (PIs) related to each target allows for measuring plant functioning. Indeed, numerous PIs have been developed over the years to assess wastewater treatment performance.

Extensive research among published literature showed different PIs with the potential to be applied to integrated MBR models regarding several important control strategies during plant management. Some emerged to meet an MBR specific necessity, while others arose as a solution for CAS processes (as well as for anaerobic systems) and were adapted for MBRs. PIs are recommended while optimizing MBR since they can interpret operating issues and present reliable results to improve plant management. In other words, PIs can enable the manager to understand which operating variables/parameters should be assessed or undergo intervention in a decision-making process, saving time and money while solving a determined problem.

Fig. 1 summarizes the main relationships between the optimization targets and the PIs, with particular attention to their positioning within the integrated MBR model.

From Fig. 1, one can understand that numerous PIs may be applied to optimize each target. Additionally, using an integrated MBR model as the platform for the framework allows for comprehensively assessing the WWTP, as the PIs can be evaluated by considering biological, physical, and integrated features. Thus, the integrated approach may be considered a reliable tool for optimizing effluent quality, energy consumption, operating costs, GHG emissions, membrane fouling, and aeration.

The following sections contain an up-to-date compendium of performance indicators regarding effluent quality, energy consumption, operating costs, GHG emissions, membrane fouling, and aeration. The main purpose of these sections is to provide the reader with mathematical elements that could be applied to the framework of integrated models for MBR multi-objective optimization.

Still, open questions are also highlighted, showing knowledge gaps and the need for further research.

3. Performance indicators

3.1. Effluent quality

The assessment of nutrient removal was the first purpose of modelling WWTPs, which is why the mathematical modelling concerning this aspect is widespread and well-developed. Nevertheless, literature usually approaches quantitative assessment only regarding nutrient removal without addressing this issue using a performance indicator. In other words, when understanding if the effluent has more or fewer pollutants, papers usually present results in concentration or percentage. For the qualitative assessment, however, the effluent quality index (EQI) is a well-known PI applied by several researchers (Verrecht et al., 2010; Ko, 2018; among others) that considers the amount of pollutants to express the condition of the effluent before its discharge. Indeed, the application of EQI meets the plant's requirements for evaluating the produced effluent, making the demand for a quantitative indicator superfluous.

The EQI is PI based on the approach of Copp (2002), which quantifies the pollution load to a receiving water body (as kg pollution units/day or kg pollution units/treated volume). The higher the result of EQI, the worse the effluent quality (Verrecht et al., 2010). As previously mentioned, EQI was applied in various works, and its acronym may be presented in different ways in the literature (e.g., EQ, EQI, among others). Thus, this work will refer to it as EQI_{LIQ} as it relates to a liquid component. The EQI_{LIQ} is calculated as follows (Nopens et al., 2010).

$$EQI_{LIQ} = \frac{1}{T - 1000} \int_{t_0}^{t_1} \left[\sum P_k(t)\right] \cdot Q_{eff} \, dt \tag{1}$$

where t_0 indicates the initial time, t_1 the end of the simulation period, Q_{eff} is the accumulated effluent flow, dt is the time step within the simulation period, P_k is the pollutant weighted concentration of each component at time t, which is expressed according to equation (2).

$$P_k = \beta_x \cdot C_k \tag{2}$$

where β_x is the weighting factor of every single pollutant, and C_k is the pollutant concentration ($mg \bullet L^{-1}$).

The value of β_x may be proportional to the pollutant harm potential or the legal limit applied by the regional law to the effluent discharge. Hence, the applicant can choose the criterion representing a liability to interpreting EQI_{LIQ} because it can contribute to an underestimated/

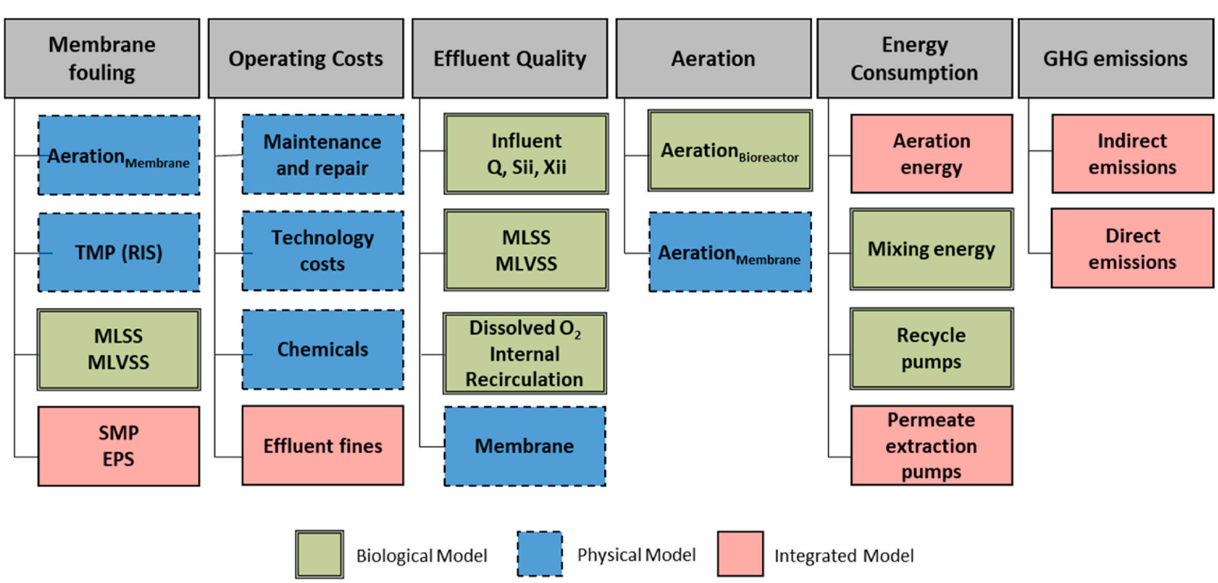

Fig. 1. Schematic representation of the framework towards MBR's optimization. Targets are presented in grey.

overestimated qualitative assessment. Despite this, several applications are reported in the literature, and β_x usually assumes similar values. For example, Gabarrón et al., 2015 used the following values for, respectively, TSS, COD, biochemical oxygen demand (BOD), total Kjeldahl nitrogen (TKN), nitric oxide (NO) and phosphorus (PO): $\beta_{TSS} = 2$, $\beta_{COD} = 1$, $\beta_{BOD} = 2$, $\beta_{TKN} = 30$, $\beta_{NO} = 10$ and $\beta_{PO} = 50$. Mannina and Cosenza (2015) employed the values reported by Vanrolleghem et al. (1996) for, respectively, COD and the soluble concentrations of ammonium (NH_4), nitrite (NO_3), nitrous oxide and PO: $\beta_{COD} = 1$, $\beta_{NH} = 20$, $\beta_{NO3} = 20$, $\beta_{N2O} = 50$ and $\beta_{PO} = 50$.

The β_{TSS} presented by Gabarrón et al., 2015 seemed a conservative measure, as the MBR is expected to retain 100% of the TSS, leading to a PTSS = 0. Considering the work of Mannina and Cosenza (2015), the value of β_{N2O} equal to β_{PO} seems to be overestimated, as N_2O represents a higher danger to the environment while in gas form, and the study considered its soluble form. Both works applied the same value for β_{COD} and β_{PO} (the only repeated component among the considered ones), and this consensus suggests that they are deemed feasible by both types of research. The nitrogenous components, however, presented a different approach. Initially, Initially, Gabarrón et al., 2015 considered TKN and NO pollutants, while Mannina and Cosenza (2015) used NH_4, NO_3, and N_2O. By evaluating both works, it is clear that the components chosen are related to those most significant within the assessed scenarios.

Nonetheless, the reason why other components were not considered is not clear, even if the concentration of a non-significant pollutant would provoke a derisory difference in the result. Even so, it is understandable that EQI_{LIQ} is calculated based on the scenario of interest using specific weighting factors because it is impossible to assume that a particular pollutant can affect different water bodies similarly. The main obstacle to this is that the absence of specific components in the equation hampers the possibility of comparing different results.

Even though some details must be defined, the EQI_{LIQ} has shown great potential in optimizing MBRs. Among several other results, Gabarrón et al., 2015 found that the lowest EQI_{LIQ} (i.e., the higher effluent quality) were correlated with the highest recirculation rate values and, consequently, with the highest pumping costs. Thus, the improvement of effluent quality corresponded to a higher operating cost. This result confirms that MBRs have a higher associated cost but also indicates a window of opportunity for plant optimization, as using an optimal recirculation rate can guarantee the best effluent quality with the minimal possible cost.

All the above PIs mainly refer to the "standard" pollution factors. New frontiers may consist of modelling (and PI definition) of emerging contaminants, given the demonstrated effect of process conditions on their removal and the advantages of MBRs vs CAS, shown by advanced monitoring techniques (Bertanza et al., 2011).

3.2. Energy consumption

As reported by Sun et al. (2016), specific energy consumption in an MBR plant has been cut these last ten years to reach 0.39 kWh·m^{-3} in Japan (Itokawa et al., 2014) and Singapore (Tao et al., 2010), 0.50 kWh·m^{-3} as an average value in China (Xiao et al., 2014), and between 0.65, 0.8 and 2.4 kWh·m^{-3} in Europe (Barillon et al., 2013; Krzeminski et al., 2012).

Different PIs can be found in the literature representing MBR's energy assessment (Maere et al., 2011; Mannina et al., 2019; among others), but they all present the same core: to assess the energy required by the pumping system. The variations observed are usually related to the boundaries considered by this system, i.e., the assessment can comprise only the air blowers or can be expanded to include recycle pumps, mixers and permeate extraction. In the end, the complete PI for the energy demand (ED) will be the one considering the highest amount of features related to power consumption, but this does not mean that all MBR scenarios need such a comprehensive approach.

Maere et al. (2011) modelled the total power requirement (PR, as kWh·m^{-3}) of an MBR using a Benchmark Simulation Model (BSM) applied to it, as presented in equation (3).

$$PR = AE + PE + ME \tag{3}$$

Where AE (as kWh·m^{-3}) is the aeration energy, PE (as kWh·m^{-3}) represents the energy of the sludge recycle pumps and ME (as kWh·m^{-3}) is the energy used for mixing the anoxic, aerobic tanks and membrane tanks.

The estimation of ME was retrieved from values provided by Metcalf and Eddy (2003). AE was split into the contributions from fine bubble aeration in the bioreactors ($AE_{bioreactor}$) and coarse bubble aeration in the membrane unit ($AE_{membrane}$). Both aerations were calculated according to equation (4) by the integration of the expression for power requirement for adiabatic compression provided by Tchobanoglous et al. (2003) during the evaluation period t:

$$AE = \frac{24}{T} \cdot \int_0^T \frac{w(t) \cdot R \cdot T}{c_{si} \cdot n \cdot e} \cdot \left[\left(\frac{p_2}{p_1} \right)^n - 1 \right] \cdot dt \tag{4}$$

where w is the mass flow of air (kg·s^{-1}) in a time t; R is the gas constant (equal to 8.314 kJ kmol^{-1}·K^{-1}); T is the absolute temperature (′C); p_1 and p_2 are the absolute inlet pressure and absolute outlet pressure (atm), respectively; c_{si} is a constant according to the International System of Units (equal to 29.7); n is a constant for air (equal to 0.283); and e is the blower efficiency (equal to 0.5). $AE_{bioreactor}$ and $AE_{membrane}$ were summed to provide the final AE.

The pumping energy considered three pump sludge flows (PS, as kWh·m^{-3}): the internal nitrate recirculation flow (Q_{R1} - m^3·d^{-1}), the waste flow (Q_{R2} - m^3·d^{-1}) and the return activated sludge flow (Q_{was} - m^3·d^{-1}). In addition, PE considered the permeate extraction (P_{EFF}) as a constant value calculated the same way as the sludge flows. The paper did not present the exact equation for these four features.

Mannina et al. (2019) calculated eD in a similar way to Maere et al. (2011). The aeration energy was estimated similarly but nominated as P_w instead of AE. The main differences between both works are that Mannina et al. (2019) did not consider the mixing energy of the four reactors, and P_{EFF} (as kWh/m^3) was calculated with a different equation, as follows:

$$P_{EFF} = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \frac{TMP \cdot Q_{eff}(t)}{3600 \cdot \eta} \cdot dt \tag{5}$$

where TMP is the transmembrane pressure; Q_{eff} is the accumulated effluent flow in a time t; η is the permeate pump efficiency, and dt is the simulation period.

Although Maere et al. (2011) did not present the equation used for P_S, Mannina et al. (2019) presented an equation (6) that considers the same three sludge flows as the first one.

$$P_S = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} 0.004 \cdot (Q_{R1} \cdot 0.06 + Q_{R2} \cdot 0.06 + Q_{WAS} \cdot 0.06) \cdot dt \tag{6}$$

where Q_{R1}, Q_{R2}, and Q_{WAS} represent the same acronyms mentioned while depicting the work of Maere et al. (2011). The values of 0.004 and 0.006 were used to convert the wastewater flow rate into kWh.

In the end, Mannina et al. (2019) calculated PR as shown in equation (7):

$$PR = P_W + P_{EFF} + P_S \tag{7}$$

Thus, for the sake of completeness, it could be said that a more comprehensive PR could be calculated as follows:

$$PR = AE + ME + P_{EFF} + P_S \tag{8}$$

These three ways of estimating PR represent several approved literature findings (cf. Metcalf and Eddy, 2003 or Henze et al., 2006 among others) which explain why they are similar and can be found in other published works (Verrecht et al., 2010; Mannina and Cosenza, 2013, 2015; among others). In addition, both works stated that PR presented realistic results for the assessed scenarios and contributed to better estimating operating costs. The fact that AE presented the highest results in both works led to the understanding that optimal aeration must be pursued to reduce the plant's energy demand while maintaining good nitrification and denitrification levels. This is, indeed, a well-known issue, which led to the development of "smart" aeration control strategies of nitrification reactors of biological WWTPs (e.g., among those based on fuzzy logic: Kalker et al., 1999; Fiter et al., 2005; Baroni et al., 2006; Ruano et al., 2024).

3.3. Operating costs

Performing a full cost analysis of an MBR is challenging because the plant has its specificities (as pointed out in Bertanza et al., 2017). Thus, before establishing a model that can calculate MBR's associated costs, it is necessary to define which boundaries shall be considered, i.e., whether the assessment wants to address economic issues considering a full-scale MBR or some specific features regarding the treatment.

OPEX is a cost indicator that can be used to determine energy and chemical demand, critical component replacement, fines related to wastewater discharges, and other items (e.g., labor and servicing) (Judd and Judd, 2011; Verrecht et al., 2010; Yang et al., 2017). On the other hand, CAPEX usually includes equipment, installation services (e.g., civil, mechanical and electrical services), and land costs (Verrecht et al., 2010; Yang et al., 2017) if the analysis is limited to the wastewater treatment process. Indeed, it is known that sludge treatment and disposal may account for half of total operation costs. Both costs can be combined to provide the net present value (NPV), which accounts for the economic profitability of the MBR investment/utilization over its lifetime. Equation (9) depicts the calculation of NPV by considering the values of OPEX and CAPEX (Verrecht et al., 2010).

$$NPV = \sum_{t=0}^{T} \frac{CAPEX_t + OPEX_t}{(i+1)^t} \tag{9}$$

where i represents the discount rate or the return net that could be earned along with the plant functioning, the sum of CAPEX and OPEX represents the net cash inflow-outflow during the time period t, and T is the time horizon of the project assessed. T usually varies from 20 to 30 years to represent the whole WWTP lifetime. The available literature did not present a specific equation for obtaining the values of CAPEX and OPEX, but a proper definition is provided in the following paragraphs.

The NVP can be used to assess MBR's costs, and its great potential is to show the advantages of investing in a robust technology (i.e., CAPEX), which may lead to a decrease in maintenance and repair costs (i.e., OPEX) and an increase in effluent quality. Despite the widespread application of the NPV, other methods may be used to perform an economic assessment of MBRs. For example, Maurer (2009) introduced the specific net present value (SNPV), which expresses plant's average costs. One is the growth rate and plant utilization over the planning horizon, factors excluded from a standard NPV approach. In other words, using SNPV can estimate the additional CAPEX for the staged expansion of a treatment plant. Equation (10) depicts the SNPV proposed by Maurer (2009), representing the NPV per service unit or population equivalent (PE).

$$SNPV = \frac{NPV}{\frac{1}{T_p}\int_0^{T_p} P_t \cdot dt} \tag{10}$$

where Tp represents the planning horizon (years) and NPV is the present value of total expenses, which, in this work, was calculated as the sum of CAPEX and OPEX. Pt represents the demand (service unit or PE) at a time dt and it is estimated as follows:

$$P_t = P_0 \cdot e^{\lambda \cdot t} \tag{11}$$

where P_0 is the population equivalents at time 0, λ is the growth rate of the population equivalents, and t is the time period.

The author applied the SNPV to an MBR-based system and obtained the OPEX, which clearly represents the economic weakness of membrane-based wastewater treatment. Finally, the manuscript stated that the advantage of SNPV over NPV is better observed when there is a need for the plant's rapid growth. It can be said that SNPV is strongly dependent on NPV; thus, its use is recommended in demanding growth situations where customer costs must be minimized. In addition to those mentioned above, the literature contains other approaches for estimating CAPEX, OPEX, and, consequently, SNVP (Maurer, 2009).

As seen by the several PIs previously presented, the economic assessment of an MBR can be a difficult task. For this reason, some researchers proposed a more simplified approach that considers the three main contributors to MBR's operating cost: the costs related to the energy demand required for aeration purposes, recycle pumps and permeate extraction; costs due to chemical consumptions for membrane cleaning; and those due to effluent fines applied for the mass of pollutants discharged (Guerrero et al., 2012; Mannina and Cosenza, 2015). Mannina and Cosenza (2015) presented equation (12) based on the previous works of Vanrolleghem and Gillot (2002) to estimate the total operating costs (TOC, as euro/treated volume).

$$TOC = CC + EF + PR \cdot \gamma_e \tag{12}$$

where PR is related to the power requirement (as euro/treated volume), as presented in equation (8); γ_e is associated with the cost of 1 kWh; CC corresponds with the chemicals consumption for membrane cleaning (as euro/treated volume); and EF are the effluent fines (as euro/treated volume). It is important to highlight that this equation does not consider the costs related to control strategy (automation and sensors), as they are location-dependent (Vanrolleghem and Gillot, 2002).

CC is important for membrane cleaning and must be considered as one of the most common strategies to reduce membrane fouling (Verrecht et al., 2008; Zuthi et al., 2012; Lee et al., 2013). For the estimation of CC, Mannina and Cosenza (2015) considered a typical membrane cleaning protocol including a solution composed of 500 ppm of sodium hypochlorite (NaOCl) and 2000 ppm of citric acid, with a value of 0.48 € per chemical cleaning. In this case, the chemical cleanings were considered to be held when the TMP reached a value higher than 60 kPa, by the manufacturer, which would contribute to a decrease in membrane efficiency and enhanced energy consumption for permeate extraction.

Some liabilities were reported in the literature regarding the use of NaOCl during MBR chemical cleaning, which is why other types of substances were reported as being able to perform membrane cleaning (e.g., nitric oxide) (Barnes et al., 2015; Jo et al., 2019). Thus, the CC cost estimation must consider which chemical is recommended for the specific cleaning process.

The EF is calculated considering the costs for effluent discharge within and without the limits established by the law (Vanrolleghem et al., 1996; Mannina and Cosenza, 2015). Hence, the effluent concentration (C_j^{EFF}) is compared with the effluent limits ($C_{L,j}$) for each relevant pollutant j during the assessment period (t_2-t_1), as shown in the following equation:

$$EF = \frac{1}{t_2 - t_1} \cdot \int_{t_1}^{t_2} \left[\frac{1}{Q_{IN}} \cdot \left(\sum_{j=1}^{n} \left(Q_{eff} \cdot \Delta\alpha_j \cdot C_j^{EFF} + Q_{eff} \cdot \left[\beta_{0,j} + \left(C_j^{EFF} - C_{L,j} \right) \cdot (\Delta\beta_j - \Delta\alpha_j) \right] \right) \cdot \left(Heaviside \cdot \left(C_j^{EFF} - C_{L,j} \right) \right) \right) \right] \cdot dt \tag{13}$$

where Q_{IN} and Q_{eff} are, respectively, the influent and effluent flow; Δa_j is the slope of the curve EF versus C_j^{EFF}, when $C_j^{EFF} < C_{L,j}$ (which attributes a value of zero to the function Heaviside), while $\Delta\beta_j$ represents the slope of the curve EF in the opposite case (i.e., Heaviside = 1); and $\beta_{0,j}$ are the increments of fines for the case represented by Heaviside = 1 (Mannina and Cosenza, 2015). In this case, the values of C_j^{EFF} were considered equal to the ones reported by Stare et al. (2007) and $C_{L,j}$ was based on the emission limits established by the environmental legislation limits.

Considering all the PIs above, it is possible to understand that researchers made a tough effort to address MBR's economic assessment. NPV and TOC can be regarded as comprehensive when addressing MBR's lifespan and performance costs. Applying both before implementing an MBR could provide important data to base decision-making regarding the investment in such technology. However, a PI considering the sum of NPV and TOC would not be recommendable, as both PIs involve completely different information.

A more exhaustive estimation of OPEX should include other relevant items, such as sludge (and other residues) management costs. Process conditions may significantly affect sludge production and characteristics; likewise, sludge line rejection liquors influence the water line behaviour and performance. Therefore, efforts should be made to include these items in the PIs list due to their relevant role in decision-making (Bertanza et al., 2015, 2016; Svanström et al., 2014).

3.4. Aeration

The importance of aeration for an MBR is related to several aspects previously discussed (i.e., effluent quality, fouling mitigation, indirect emissions, and operating costs). For example, the aeration of membrane modules is known as one of the reasons why MBRs are a higher-cost technology compared to conventional systems due to the higher energy demand for the aeration blowers (Wu and He, 2012; Capodici et al., 2015). This fact also implicates an increase in indirect GHG emissions (Mannina et al., 2019), which shows that its optimization can affect the whole MBR system.

The major obstacle related to this aspect is that only some PIs applicable to aeration were publicized, and the most known are from ancient literature. Among the available options, the most disseminated are related to the biological treatment and were mostly applied to CAS or only to the biological reactor without influencing the MBR. Among them, it can be mentioned the oxygen transfer rate (OTR, as $kgO_2{\cdot}h^{-1}$), the aeration efficiency (AEFF, as $kgO_2{\cdot}kWh^{-1}$), the oxygen transfer efficiency (OTE, as %) and the oxygen uptake rate (OUR, as $mg{\cdot}L^{-1}{\cdot}h^{-1}$). OTR, AEFF, and OTE are related to the oxygen mass transfer, while OUR is related to dissolved oxygen (DO) consumption.

More details regarding these PIs can be found in the literature (Henze et al., 2006; Trussell et al., 2007; Pittoors et al., 2014). However, it is important to mention that several studies reported these PIs with different nominations, such as standard oxygen transfer rate (SOTR), standard oxygen transfer efficiency (SOTE) and standard aeration efficiency (SAEFF) (Naessens et al., 2012; Suh et al., 2013; Ko, 2018). These standardized PIs consider process standard conditions instead of site-specific ones to avoid mistakes while interpreting results. Such standard conditions are zero DO, zero salinity and 20 °C and 1 atm (Henze et al., 2006). In addition, the application of only one aeration PI is not considered enough as a method to evaluate and predict the performance of a plant configuration. Indeed, from a control point of view, minimizing energy without explicitly taking into account at least one performance criterion or constraint simply does not make sense. To be properly posed, any control problem must consider both cost criteria (in this case, linked to system operation, e.g. the energy demand for system oxygenation) and at least one performance criterion (or constraints), e.g. the desired level of rejection. Thus, considering the connection among them, it would be recommendable to apply more than one to obtain a more comprehensive interpretation of the phenomena related to aeration.

Another interesting PI to be considered when it comes to aeration aspects related to biological treatment is the oxygen-to-total-Kjeldahl-nitrogen ratio (R_{ON}) (Boiocchi et al., 2017; Mannina et al., 2020). RON provides a relation between the amount of oxygen supplied by the aeration system versus the amount of Total Kjeldahl Nitrogen (TKN) in the influent to understand how much of the oxygen provided to the system was used to oxidize the influent ammonium. R_{ON} is a reliable way to obtain an optimal oxygen supply reference and is calculated in equation (14).

$$R_{ON} = \frac{\sum_{i=1}^{n} k_L\alpha_{AER,i}\cdot V_{AER,I}\cdot\left(SO_{2,SAT,i} - SO_{2,AER,i}\right)}{Q_{in}\cdot S_{NH,in}} \tag{14}$$

where $k_La_{AER,i}$ is the oxygen mass transfer coefficient of the aerated tank i; $V_{AER,i}$ is the volume of the aerobic tank i; $SO_{2,SAT,i}$ is the oxygen saturation concentration of the aerobic tank i; $SO_{2,AER,i}$ is the oxygen concentration in the aerobic tank i; Q_{in} is the inlet flow rate fed to the biological zone; and $S_{NH,in}$ is the inlet ammonium nitrogen fed to the biological zone. The sum ($\sum$) represented in the equation is related to all aerated sections (i.e., aerobic and membrane reactors).

RON was also used by Vangsgaard et al. (2012), as it typically indicates the aeration regime of the treatment plant. It must be highlighted that Boiocchi et al. (2017) applied R_{ON} to a CAS system (anoxic and aerobic zones), whilst Mannina et al. (2019) adapted it for an MBR integrated model (anaerobic, anoxic and aerobic zones and a side-stream membrane bioreactor). However, the application of R_{ON} to an MBR did not affect its calculation. From the work of Mannina et al. (2019), it was possible to notice that only the features related to the aerobic reactor substantially affected R_{ON}.

Extensive research among published literature indicates the absence of a PI to assess the effects of aeration over membrane fouling. Indeed, as shown in the previous section, PIs related to fouling are mostly related to membrane resistance and solids concentration in view of assessing phenomena such as cake deposition, pore blocking and clogging, reversible and irreversible fouling, among others. However, the role of aeration over fouling should be appropriately analysed since air scouring is responsible for the shear rate at the membrane surface and the particle back transport into the bulk fluid. A comprehensive assessment regarding such aspects may provide tools to help augment membrane lifespan and reduce fouling (Armbruster et al., 2019). Even though no specific PI was found during this research, the literature indicates the shear intensity of the fluid turbulence (G) as an alternative PI able to provide a correlation between aeration and cake formation/membrane fouling (Mannina et al., 2011).

The estimation of G (s^{-1}) is based on the cross-sectional approach (Li and Wang, 2006), which divides the membrane surface into a number i of equal horizontal sections to assess the reduction of fluid shear caused by aeration turbulence over the particles deposited on the membrane surface. The cross-sectional approach considers that fouling is not uniformly distributed on the membrane area surface due to the action of the air blowers (Chu and Li, 2005); thus, the uneven distribution leads to a different sludge cake deposition in each membrane horizontal sections (i) (Li and Wang, 2006). In the end, G_i (equation (15)) is related to the turbulence effect suffered by the particles deposited on each i section of the membrane. In this case, it is assumed that the higher the section, the smaller the turbulence suffered by the particles (Mannina et al., 2011).

$$G_i = \left|\begin{array}{l} \left[0.1 + 0.45\cdot\left(1+sin\dfrac{(2\varepsilon_i - \varepsilon_a)\cdot\pi}{2\varepsilon_a}\right]\cdot\sqrt{\dfrac{\rho_s\cdot g\cdot q_a}{\mu_s}};\ \varepsilon_i < \varepsilon_a \\ \sqrt{\dfrac{\rho_s\cdot g\cdot q_a}{\mu_s}};\ \varepsilon_i \geq \varepsilon_a \end{array}\right. \tag{15}$$

where q_a ($m^{-2}{\cdot}s^{-1}$) represents the air flow rate, g represents the gravity acceleration ($m{\cdot}s^{-2}$) and ρs represents the sludge density ($kg{\cdot}m^{-3}$). The parameter ε_i (m) is related to the fraction of the membrane surface nearest to the aerator (i.e. where the G_i is more intense), and ε_a (m) regards the membrane surface where the turbulence effect is reduced. The sludge viscosity (μ_s as Pa·s) is reported in equation (16) as a function of water viscosity (μ_w, as Pa·s) and the MLSS concentration.

$$\mu_s = \mu_w \cdot 1.05 e^{0.08 \cdot MLSS} \tag{16}$$

As shown in equation (15), G_i will assume a different value for every section i to represent the uneven effect of aeration turbulence along the membrane length. From this, it may be assumed that G_i would only be applicable for models, considering that the shear force is not uniformly distributed. However, for more simplified models, i.e., that consider a uniform turbulence effect along each i-section, the expression of G can be simplified as follows (Suh et al., 2013):

$$G = \sqrt{\frac{\rho_s \cdot g \cdot q_a}{\mu_s}} \tag{17}$$

Mannina et al. (2011) and Suh et al. (2013) used the value of G to obtain the mass of solids attached and detached to the membrane during the suction phase by Li and Wang's (2006) approach. The attachment considered the forces of adhesion (i.e., the diagonal trajectory towards the membrane surface during the permeate suction) and lifting (i.e., the force exerted by the aeration, which directs the particle upwards within the reactor, allowing the particle to deposit itself along the whole membrane surface). On the other hand, the detachment regards the force related to the backwashing flux. In the end, it is possible to obtain the thickness of the dynamic sludge cake layer (i.e., the reversible cake that can be removed by aeration) and the irreversible cake's thickness. From this application, G as a PI may be applicable to correlate the aeration intensity with the formation of reversible and irreversible fouling. However, since G depends on other information (e.g., adhesion and lifting forces, probability of cake deposition), it must be coupled with other calculations to provide a result that can be interpreted in terms of membrane fouling.

3.5. GHG emissions

The GHG emitted from MBRs are mainly CO_2 and N_2O (Daelman et al., 2015; Lorenzo-Toja et al., 2016; Mannina et al., 2016, 2018, 2019). CO_2 is mainly formed by bacteria's metabolic activities (i.e., direct emissions). It may also be formed while converting the energy and chemical consumption in terms of carbon equivalent ($CO_{2,eq}$) (i.e., as indirect emissions) (Corominas et al., 2012; Bao et al., 2016). The N_2O is mainly produced during the biological conversion of nitrogen into nitrogen gas (N_2) through the nitrification and denitrification processes (Kampschreur et al., 2009). The pathways for NO formation from WWTP are extensively detailed in the literature (Wunderlin et al., 2012; Pocquet et al., 2016; Ribera-Guardia et al., 2019), and the importance that has been given to this matter shows how important it is to have tools able to correctly estimate N_2O emissions and help in its mitigation (Mannina et al., 2019).

The CO_2 is formed during an intrinsic part of the wastewater treatment (i.e., bacteria metabolic activities), so its emissions can be reduced but hardly prevented. Most of the N_2O is formed as an intermediate product of an incomplete reaction. This fact led researchers to question if optimizing wastewater treatment in terms of ammonium could reduce the emissions of N_2O (Monteith et al., 2005). For this reason, various quantification methods are reported in the literature (Shahabadi et al., 2010; Pan et al., 2011; Rodriguez-Garcia et al., 2012; among others) to promote a solution for the GHG emissions from MBRs, especially regarding N_2O.

CO_2 and N_2O are easily soluble in water. Henry's law constants of CO_2 and N_2O are 34 and 24 mM atm^{-1} (at 25 °C and 0% salinity), respectively (Weiss and Price, 1980), which is considered relatively high in comparison to that of O_2 (1.3 mM atm^{-1}, at 25 °C and 0% salinity). Therefore, both gases are known to accumulate in the liquid phase during wastewater treatment. Considering this concept and based on the work of Mannina and Cosenza (2015), Mannina et al. (2019) calculated the stripping of CO_2 and N_2O off-gas from their liquid forms to obtain the amount of GHG that can be stripped due to aeration. The quantification of GHG emission with mass transfer from liquid to gas is well spread in the literature (Daelman et al., 2015; Marques et al., 2016).

Despite its high GWP (28 over 100 years) (IPCC, 2014), CH_4 is the less studied GHG when it comes to MBRs because its production is mainly observed when anaerobic processes are implemented (Mannina et al., 2018). This, again, stresses the importance of including the sludge treatment within overall assessment procedures, as sludge may be stabilized via the anaerobic process. Indeed, the superficial assessment observed while quantifying CH_4 emissions from MBRs is related to the fact that membrane studies are often looking for answers regarding the waterline boundaries, which are those most influenced by MBRs, whilst approximately 72% of CH_4 emissions are related to the sludge lines (Nguyen et al., 2019). Thus, its emission is usually accounted for in full-scale processes containing an anaerobic digester or when sludge handling is considered part of the assessment.

Mannina et al. (2019) applied equations (18) and (19) to calculate the total direct emissions (DE) and total indirect emissions (IE), respectively. Due to the boundaries considered by the study, the emissions of CH_4 were not inserted in the DE equation.

$$DE = Offgas_{CO_2} + \left(Offgas_{N_2O} \cdot 265\right) \tag{18}$$

$$IE = \left(P_w + P_{eff} + P_s\right) \cdot 0.245 \tag{19}$$

where DE and IE were given as $kgCO_{2,eq}$•m^{-3}. IE was calculated by considering the concepts of P_w, P_{eff} and P_s presented in section 3.2, which represents the total energy demand of the system (eD). The numbers 265 $kgCO_{2,\,eq}$ and 0.245 $kgCO_2$ kWh^{-1} were conversion factors. The sum of DE and IE represents the quantification of the GHG emitted by the plant. It must be highlighted that, in case of a plant-wide assessment, the emissions from the sludge line should be included to obtain the total results of DE and IE.

Mannina et al. (2019) reported that DE and EQI_{GAS} presented similar behaviors, while IE presented a similar behavior to PR and TOC (see equations (8) and (12), respectively). It is possible to understand that the EQI_{GAS} represents a reliable PI due to its similarity with DE, even though the weighting factors applied for its calculations were based on a subjective criterion. However, it is recommended to reconsider the values of β_{CO2} and β_{N2O}, as both gasses were expressed as having a similar potential to threaten the atmosphere, which does not depict the reality (IPCC, 2014). The fact that IE, PR, and TOC are similar illustrates that reducing MBR's energy consumption may be considered a priority during MBR's optimization.

For completeness, Mannina et al. (2019) presented a modified version of the EQI (see equation (1)) to include gas emissions. The EQI_{GAS} represents a qualitative assessment of gas emissions, considering the potential of CO_2 and N_2O to harm the atmosphere. The estimation of this PI is quite similar to the EQI_{LIQ}, as shown in equation (20).

$$EQI_{GAS} = \frac{1}{T - 1000} \int_{t_0}^{t_1} \left(\beta_{CO_2} \cdot Offgas_{CO_2} + \beta_{N_2O} \cdot Offgas_{N_2O}\right) \cdot Q_{eff} dt \tag{20}$$

where $Offgas_{N2O}$ and $Offgas_{CO2}$ are related to the gas emitted by the plant and β_{CO2} and β_{N2O} are the weighting factors of, respectively, CO_2 and N_2O. In this case, β_{CO2} and β_{N2O} were equal to 50. Q_{eff} is the accumulated effluent flow, and dt is the simulation period. Both weighting values were chosen based on the author's experience with the lack of similar values in the literature.

3.6. Membrane fouling

The formation of membrane fouling is mainly attributed to the undesirable deposition and accumulation of organic, inorganic and biological particles on the membrane surface (Zhang and Jiang, 2019; Zhang et al., 2021). This reduces permeate flux and increases TMP lead, reducing productivity, increasing treatment costs, and reducing membrane lifespan (Zuthi et al., 2012). A more conceptual overview of the phenomena leading to membrane fouling and the reduction of MBR energy consumption can be found in the literature (Jang et al., 2006; Hamedi et al., 2019; Wang et al., 2024).

Even though several studies have included this aspect as the main topic, membrane fouling is still an "open challenge" when optimizing MBRs. Many strategies have been tried to reduce fouling. The main similarity among them is that they require direct intervention on the membrane module, which is not always possible due to several operational reasons. In this case, the optimization through applying an integrated mathematical model associated with a proper PI can provide a faster response and allow managers to identify which operating variable needs an intervention before acting on the process or the equipment. The main problem is that a few options are available in the literature.

The first assessment of membrane fouling with mathematical modelling was made through the resistances in series (RIS) models (Psoch and Schiewer, 2006; Rafiei et al., 2014; Di Bella et al., 2018, among others). However, the calculation of the resistance-in-series relates to the membrane resistance, which is more applicable as a control parameter than a PI. Among the available options of PIs, the modified fouling index (MFI) is even used to predict fouling formation on the membrane. It is considered a reliable sludge filterability indicator for investigating the potential of fouling formation by considering the MLSS characteristics and the physical treatment configuration (Sun et al., 2019). MFI (given as $s \cdot L^{-1}$) was derived by Schippers and Verdouw (1980), and its main concept relies on the fact that fouling mechanisms occur in the order of pore blocking, cake/gel filtration and cake/gel blocking (Schippers and Verdouw, 1980; Salinas-Rodriguez et al., 2015; Jin et al., 2017). In addition, its main assumption is that the amount of matter deposited on the surface of the membrane is proportional to the permeated volume. Thus, MFI is defined as the gradient of the linear region found by the slope of the ratio between the filtration time (t_f, given as seconds) and the permeated volume (V, as liters) versus V, as shown in equation (21) (Jin et al., 2017)

$$MFI = \frac{t_f}{V} = \frac{\mu R_m}{\Delta PA} + \frac{\mu I}{2\Delta PA^2} \cdot V \tag{21}$$

where ΔP is the applied pressure (as $N \cdot m^{-2}$), μ represents the MLSS viscosity (as $N \cdot s \cdot m^{-2}$), R_m is the membrane resistance (m^{-1}), A is the membrane surface area (m^2), and I is the fouling index, which is determined as shown in equation (22).

$$I = \alpha \cdot C \tag{22}$$

where α is the cake resistance, and C is the solids concentration.

MFI final result shows a linear correlation between the matter concentration (colloidal and suspended) that attaches to the membrane. The MFI is very often applied to membranes with pore sizes of 0.45 μm (MFI0.45). Still, it was also adapted for membranes that perform ultrafiltration (MFI-UF), nanofiltration (MFI-NF) and reverse osmosis (MFI-RO) as the MFI0.45 was not considered adequate to predict cake formation for different pore sizes (Salinas-Rodriguez et al., 2015; Jin et al., 2017; Sun et al., 2019; among others).

Other approaches can be found in the literature in view of obtaining the value of MFI (Ju et al., 2015; Harouna et al., 2019; Mannina et al., 2019). Despite how widespread MFI is nowadays as a PI for assessing membrane fouling, some concerns are reported in the literature regarding its representativity when a real application is considered. The dimension of MFI (time/volume) is one of the objects of criticism since MFI seems to group many dimensional parameters that must ultimately explain a relationship between time and volume, making the interaction caused by the membrane resistance or the solids concentration a secondary issue. For this reason, the Dimensionless Fouling Index (DFI) was introduced to overcome the issue related to the measurement unit described by the MFI and to allow other important parameters to be accounted for as having more effective participation while assessing membrane fouling. DFI represents the ratio between the membrane resistance and the cake due to the TSS concentration by Equation (23).

$$DFI = \frac{R_T^2}{2P_{TSS} r_{sc}} \tag{23}$$

where R_T is the total membrane resistance (m^{-1}), to properly describe the membrane fouling, it was calculated as proposed by Judd and Judd (2011). The other acronyms of equation (23) were described along with equation (21). In this case, r_{sc} can be calculated as Mannina et al. (2011) suggested.

Mannina et al. (2019) applied DFI to assess the membrane fouling of a hypothetical plant-wide MBR plant. They used an integrated process-based mathematical model to the plant, and the results showed a strong correlation between DFI and solids concentration (including SMP concentration).

Once defined, coupled with an integrated model, Pis can be monitored and estimated, possibly online, within a "plant-wide optimization" framework.

4. Integrated MBR models towards optimization

As mentioned, MBR optimization may be achieved by using performance indicators after establishing optimization targets. Although much information was published regarding PI and MBR modelling, only a few works combine both aspects to optimize the whole MBR system. The main works published in the literature concerning this subject, along with their main findings, are summarized here below and synthesized in Table 1.

Table 1
Optimization of MBR through integrated model.

Reference	Optimization method	PIs	Results
Maere et al. (2011)	Operating and control strategies – PI controllers	EQI, EC, operating costs	Proof of concept for identifying control strategies that would minimize operating costs without compromising the effluent quality
Gabarrón et al. (2015)	Scenarios analysis of control strategies	N removal rate, for low operating cost	Influence of the DO set point
Ko (2018)	MINLP	EQI_{liq}, energy	Influence of Recycle ratio, biological aeration flowrate
Mannina et al. (2019)	Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS)	EQI_{LIQ}, EQI_{GAS}, GHG emissions, RON, TOC, EC, effluent fines …	48% reduction of TOC, 10% reduction of direct GHG emissions. Not possible to optimize all the PIs
Nam et al. (2021)	Dual-objective optimization, Harmony Search	$J_{biological}$ (AE, EQI_{liq}) + $J_{physical}$ (PErmeation, TMP, Water Production)	Up to 12% reduction of EC while maintaining effluent quality. Optimized physical cleaning duration decreased PE by up to 17%, extended membrane life span by 17 days …

- The work of Maere et al. (2011) was one of the first to consider the possibility of optimizing an MBR system using modelling techniques. The work used a benchmark simulation model for an MBR (BSM-MBR) to evaluate operating and control strategies to enhance effluent quality and reduce energy consumption and operating costs. The results presented included two closed-loops, but it is clearly stated that these results are just proof of concept for the simulator and that it is up to the users to use any sets of actuators/sensors and PIs. The BSM-MBR model was coupled with a dedicated aeration model to incorporate the effects of sludge concentrations and the aeration efficiency. On the other hand, SRT, high biomass concentration, and extensive aeration contributed to improved ammonium removal at the expense of a high operating cost. The model itself could not provide an optimized result for the aeration; thus, a closed-loop simulation was applied as proof of concept for identifying control strategies that would better influence lowering operating costs without compromising the effluent quality.
- Gabarrón et al. (2015) applied a mechanistic integrated model to a full-scale MBR to simulate viable optimization strategies for improving effluent quality and reducing operating costs. To do so, the performance indicators developed for the BSM were used to estimate the EQI. At the same time, the TOC was calculated by considering the energy required for aeration and pumping procedures, as well as sludge production. In this study, the actuators were the recirculation rates between the different components of the system and the aeration rates in the aerobic tank. The authors found room for improving nitrogen removal efficiency by assessing the plant's performance, especially during denitrification. In addition, modelling results showed that air blowers for biological aeration were responsible for up to 55% of the total energy consumption, which made it imperative to promote its optimization. The use of BSM, in this case, is related to the assessment of the plant, considering not only the biological and physical treatment but also its full-scale composition. For this reason, the operating costs included the amount of sludge produced.
- Castillo et al. (2016) coupled a multi-criteria analysis to an integrated MBR model to generate a ranked short-list of possible treatments for three scenarios (which included different types of wastewater treatment). An uncertainty analysis was further applied to increase the robustness of the decision. Results showed that the MBR was the optimal treatment and the most robust solution under influent uncertainties and tighter effluent limits. The mathematical modelling applied for optimization was considered reliable when selecting the most appropriate treatment alternative.
- Ko (2018) applied an integrated model to optimize the design of an MBR system composed of two anoxic tanks, two aerobic tanks, and one immersed membrane tank. This application aimed to assess the MBR functioning with different configurations, volumes, and flow rates to obtain the most reasonable plant configuration. A mixed-integer non-linear programming (MINLP) optimization technique was used to determine the optimal design and set of operating variables for the plant operation. Results showed a direct influence of the recycle ratio on EQI_{LIQ}. Additionally, a decrease in the recycling and aeration flow rates resulted in an optimized value of EQI_{LIQ}, pump energy, and aeration energy. Membrane fouling was not considered during this optimization, but the author recommended its inclusion in future assessments.
- Mannina et al. (2019) applied an integrated dynamic model to an MBR pilot plant to optimize its functioning. The model applied was calibrated and validated in previous works. The following PIs were used as a reference during the optimization process: EQILIQ, EQI_{GAS}, GHG direct and indirect emissions, RON, TOC, energy demand, and effluent fines, among others. Model application comprehended 5000 simulations with different operating parameters to understand their influence over the PI outputs. A global sensitivity analysis (Extended-FAST method) was employed to understand the effect of each variable on the PIs. After this step, an optimization technique named Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) was applied to the most sensitive results in view of identifying the set of parameters (amongst the applied ones) that provided the optimal result to be adopted by the plant under study. Model simulation run with the select set of parameters allowed a 48% reduction in operational costs and a 10% reduction in direct emissions. The optimization also made it easier to understand that, to optimize some PIs, some others may be negatively affected. Thus, the important aspect of this optimization is finding the best trade-off for proper plant operation. Also, in this study, the membrane fouling was not assessed as a PI since membrane resistance was evaluated as a RIS system.

Such works are examples of the plant-wide nature of the optimization of MBRs. In the next section, we concentrate on the online implementation of control by focusing on online membrane fouling control strategies. In such cases, integrated modelling is usually used as a virtual plant on which the membrane fouling control strategy is tested and evaluated.

5. Online integrated model-based control

While optimizing any process does not necessarily mean implementing any feedback, the particularity of online control is that it proceeds with time explicitly taking into account the actual state of the system to react to it. It is usually the case in the operation of treatment processes in highly dynamic environments. It should be noted that an MBR, by its nature, operates by alternating two phases (filtration and backwash/relaxation) and cannot be compared to other biological reactors in terms of control. Because of the total decoupling of hydraulic and solid retention times in such systems, the time response of MBR is much less than any other biological system: this is one of the specific features of MBRs that makes them excellent candidates for online control. In addition, because the main limitation to MBR functioning is membrane fouling, many online optimization and control systems are dedicated to the management of membrane fouling, giving to the online control a great potential to improve MBR functioning. The first online fouling model-based control results can be attributed to Drews et al. (2009); Busch and Marquardt (2009). Their papers dealt on the use of simple models to automatically adapt filtration/backwash length and fluxes to maximize permeability. While the papers reported in Table 2 are representative of most recent or representative available results in membrane fouling control, the reader may refer to several recent review papers for alternative fouling control methods, such as Quorum Quenching Reactors (Pang et al., 2023), scouring (Zhang et al., 2021) or in playing with process configurations to favor optimal bubble size (Wu et al., 2024), new technologies like the increasing use of Low-Pressure membranes (Ladouceur et al., 2024), the use of new sensors as Raman spectroscopy (Virtanen et al., 2018) or actuators like ultrasounds (Arefi-Oskoui et al., 2019) or still reviewing recent knowledge available on fouling mechanisms (Chang et al., 2019). Notice that the problem of online fouling control is very similar for aerobic MBRs and anaerobic MBRs: Table 2 lists some of the articles already cited in the 2018 state of the art proposed in (Ferrero et al., 2012; Robles et al., 2018), the latter one devoted explicitly to AnMBRs. Because the problem of fouling control is completely different for nanofiltration and reverse osmosis processes, we focus in Table 2 below on studies related to online fouling control methods for micro- and ultrafiltration MBR systems. Following the same idea, works reported on diafiltration membranes, where the diluent input together with fouling control parameters are usually the main controls, are not reported here: the reader can refer to (Robles et al., 2018), where some studies are reported.

The lessons learned from these papers are as follows.

Table 2
Most representative online control methods for controlling membrane fouling.

Reference	Type of MBR/model used for the virtual plant	Simulation (S) Experimentation (E)	Control method	Control objectives	Actuators
Busch et al. (2007); Busch and Marquardt (2009)	Submerged hollow fiber aerobic MBR	E	Run-To-Run control (model-based predictive control principle)	Plant operating costs	Backwash frequency and flux
Vargas et al. (2008)	Submerged tubular membrane module of PVDF	E	TMP-based control	Permeate flux	Backwash frequency
Drews et al. (2009)	Data from the literature	N/A	Recognition of pore blocking mechanism	Maximize permeability	Backflusk flux, aeration
Ferrero et al. (2011)	Submerged hollow fiber and flat sheet MBR	E	Permeability trend	Short and long term permeabilities	Aeration flow rate
Villarroel et al. (2013)	Submerged hollow fiber microfiltration	E	TMP-based control	Permeate flux	Cleaning frequency
Robles et al., 2014	Submerged hollow fiber anaerobic MBR (ultrafiltration)	S	Supervisory-control (hierarchical control with fuzzy-logic controller)	Plant operating costs	Backwash frequency and duration/ setpoints
Chan et al. (2016)	PVDF	E	Stochastic formulation of the Busch and Marquardt algorithm	Plant operating costs	Backwash frequency and flux
González et al., 2018	Hollow fiber membrane	E	Knowledge-based control (decision tree)	Regulation around a given filtration time setpoint	Permeate flux, filtration time and TMP
Kalboussi et al. (2018)	MF/UF - Resistance in series model	S	Optimal control	Volume of treated water over a period of time T	Filtration/Backwash time period
Wahab et al. (2020)	Submerged hollow fiber microfiltration	E	Neural-based internal model	Permeate flux	Permeate pump power
Aichouche et al. (2020)	MF/UF - Resistance in series model	S	Optimal control	Functioning costs	Filtration/Backwash time period
Ellouze et al. (2023)	UF	E	Optimal control	Functioning costs	Filtration/Backwash time period

- The first lesson learned from this review is that there is a very high diversity of works. Most of them use a "model-based" approach, in the sense that the authors have used a simulation tool (an integrated model, whatever its nature) to predict the fouling dynamics.
- To the author's knowledge, very few studies optimize the functioning of the whole plant (effluent quality/cost operations) and the fouling (cf. section 4). In most cases, the optimization of MBR refers either to the control i) of the biological part, notably in terms of effluent quality - controlling the process with the aeration or with the recirculation rate in the case of a plant involving several tanks (cf., for instance, Gabarrón et al., 2015; Odriozola et al., 2017; Liao et al., 2024) - or ii) of the fouling (e.g. by maximizing the permeate volume produced in a given time or by minimizing the operating cost), explicitly (or not) considering influent characteristics as disturbances to be rejected (cf. e.g. Chaaben et al., 2024), but almost never both objectives at the same time.
- Models based on AI or data-driven techniques (including neural networks) are increasingly used: the reader may refer to (Jawad et al., 2021; Bagheri et al., 2019 or Yusuf et al., 2019) for recent reviews. Very few results without online control are available (and thus, the corresponding studies are not reported in section 4). Several recent papers have highlighted the high performance of dynamic fouling prediction and suggested the use of such control methods (Prado-Rubio and Huusom, 2024; Wang and Li, 2024). However, in such a case, it should be noted that their ability to estimate PIs essential for control remains open since most techniques are dedicated to the prediction of membrane fouling properties and not necessarily all RIS available when using mechanistic-based integrated models.
- It is particularly interesting to note that most of the proposed approaches have been evaluated on real pilot plants, not on full-scale plants. Integrated models are not currently used for online fouling control; they are rather used as virtual processes to evaluate new control approaches. The real interest of integrated models is to evaluate the performance of controlled MBRs, in particular, to estimate PIs that are difficult or impossible to measure or that would be too costly to monitor online.

Evaluation and validation of plant-wide MBR systems using integrated modelling are part of prospective work. If not sure, it is also likely that data-based and AI methods will probably be coupled with physical modelling to address the intrinsic complexity of MBR systems, allowing a better understanding and control of such systems.

6. Discussion and perspectives

The integrated MBR models can provide credible estimations and allow managers to explore a variety of operating scenarios before their application on-site, avoiding waste of environmental, physical and chemical resources while optimizing operating costs, energy consumption, effluent quality, among others, that can be estimated and monitored through Pis. For this reason, a framework that uses integrated MBR modelling to optimize MBR's outputs can be considered a reliable tool, and it has already shown to provide positive results (Gabarrón et al., 2015; Ko, 2018; Mannina et al., 2019; among others). We note that there is little, if any, integration of modelling and control approaches in new technologies developed to control MBRs, such as Quorum Quenching Reactors, which technology continues to develop (Pang et al., 2023). We can imagine that such integration would lead to high-performance systems whose control issues remain unresolved for the time being.

Specifically concerning the PIs that can be applied to an integrated mathematical model in order to provide MBR optimization, one can retrieve the following considerations.

- The weighting factors applied to EQI_{LIQ} and EQI_{GAS} may represent a liability because they seem related to an empirical choice. Nevertheless, several authors have reported the use of EQI_{LIQ} as a reliable way to correlate the effluent concentration to the environment, and this link is very often required, which makes its use recommendable.
- Specifically for the gaseous index, both gases have a similar potential to threaten the atmosphere, which does not represent reality since N_2O has a GWP 265 times higher than CO_2 (IPCC, 2014). Despite this, the EQI_{GAS} can be considered a suitable PI to provide a simplified response regarding GHG direct emissions.

- Considering the GHG emissions, the most efficient way to reduce them could be by modifying some operating conditions during the treatment, which is not always possible due to the operating limitations of the installed units (Campos et al., 2016). However, the application of a mathematical model to understand which operating condition is more relevant to the GHG scenario may be the key to allowing a focused intervention that can be performed without the necessity of strongly interfering in the treatment.
- Energy demand and TOC are directly linked, and it is important to optimize both since they are considered the main reasons for the technology stagnation. Regarding aerobic MBRs, it is possible to affirm that the aeration has a large potential for optimization, and this operation is imperative since it can influence all other optimization targets. Considering the aeration as an optimization target, its main purpose is to correlate the amount of oxygen supplied to the system with the oxygen consumption by the biomass, which can allow plant owners to foresee the long-term costs of the aeration systems and the eventual necessity to meet peak oxygen demands.
- Membrane fouling still is one of the major challenges when it comes to optimizing an MBR due to the lack of understanding of the consequences that lead to it. Many aspects are already known, and there are some PIs that can be applied to foresee the membrane fouling by considering the sludge and treatment features. However, the literature still has space to provide researchers and engineers with a more comprehensive tool to consider the dynamicity surrounding the fouling phenomenon. The literature reviewed shows that most online optimization studies of MBRs rely, in fact on the optimization of the fouling itself, without taking any consideration of the biological compartment. It is expected that using integrated MBR models together with performance indicators will provide new, cost-effective ways to be applied to global optimization approaches.
- Finally, using RON as a PI is recommended for integrated MBR models when there is an interest in optimizing the biological treatment before the physical (in case of a side-stream MBR) by means of oxygen control strategies or immersed membranes coupled with aerobic tanks. Consequently, the PI is not recommended to seek a reduction of the energy demanded in side-stream MBRs, as the study by Mannina et al. (2019) did not report major changes in this case.

A major advantage of using an integrated model is optimizing both system design parameters (e.g. reactor volumes, configuration, etc.) and degrees of freedom (e.g. recirculation rates, set points for certain control variables, etc.). - all these variables are more like constants - with control variables such as aeration rates, certain recirculation or purge flow rates - more like dynamic variables.

To summarize, from the literature review reported above, and in line with the previous work realized within the IWA WG on MBR modelling, one can claim that integrated models are reliable tools to be applied to the optimization of MBR systems in allowing a realistic way of simulating such complex processes. As for well-adopted models like the ASM series or the ADM1, models used for MBR optimization should be built with a common basis, notably concerning what makes their specificity, that is, the way the biological compartment is coupled to the filtration compartment. In this sense, it is not a question of imposing a single model but of providing methodological keys to improving understanding of the models, their coupling and implementation.

CRediT authorship contribution statement

Giorgio Mannina: Writing – review & editing, Writing – original draft. **Marion Alliet:** Writing – review & editing, Writing – original draft. **Christoph Brepols:** Writing – review & editing, Writing – original draft. **Joaquim Comas:** Writing – review & editing, Writing – original draft. **Marc Heran:** Writing – review & editing, Writing – original draft. **Angel Robles:** Writing – review & editing, Writing – original draft. **Ignasi Rodriguez-Roda:** Writing – review & editing, Writing – original draft. **María Victoria Ruano:** Writing – review & editing, Writing – original draft. **Valeria Sandoval Garcia:** Writing – review & editing, Writing – original draft. **Ilse Smets:** Writing – review & editing, Writing – original draft. **Jérôme Harmand:** Writing – review & editing, Writing – original draft.

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

No data was used for the research described in the article.

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